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ATMOSPHERIC DISPERSION OF HYPERGOLIC LIQUID ROCKET FUELS, (VOLUME I OF II)

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Titan II weapons systems are charged with hypergolic liquid rocket propellants (hydrazine fuel and nitrogen tetroxide oxidizer). These same propellants are used in support of other systems, including the MX missile and the space shuttle. This effort was designed to characterize the interactions of hypergolic liquid rocket propellants and to provide information pertinent to the development of a model to describe the transport and diffusion of airborne combustion products and unreacted vapors from an accident involving these propellants.

This report is prepared in two volumes. Volume I addresses the reactions between nitrogen tetroxide and hydrazine, including the reaction products and the heat released. This information was used to determine the combustion time and the height of the resulting fireball before it cools and disperses with the air. Volume II discusses the chemical and physical interactions of the combustion products with air, and the dispersion of these products in the environment.

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PREFACE

This final report, published in two volumes, was prepared by Martin Marietta Aerospace, P.O. Box 179, Denver, Colorado 80201, under Contract F42600-81-D-1379 for the Air Force Engineering and Services Center, Engineering and Services Laboratory, Tyndall Air Force Base, Florida 32403. Efforts documented in this report were performed between June 1982 and December 1983. Major Gary Worley and 2Lt Glenn Seitchek were the AFESC/RDVS project officers.

This report has been reviewed by the Public Affairs Office (PA), and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This report has been reviewed and is approved for publication.

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INTRODUCTION

The Titan II Weapons System is deployed at sites in Arizona, Arkansas, and Kansas. Although these sites were rural when initially deployed in the 1960s, land development and population expansion has gradually encroached upon many of the current sites. Because the Titan II Weapons System is charged with toxic hypergolic liquid rocket propellants (hydrazine fuels and nitrogen tetroxide oxidizer), the civilian population near these sites must be protected from accidental atmospheric releases of these toxic propellants in the event of a transportation, handling, or storage accident. In addition, these same propellants are used in support of other operational and planned weapons system (e.g., Minutemen III and M-X missile) and space launch vehicles (e.g., Space Shuttle).

Procedures for predicting toxic vapor corridors for an accidental release of either hydrazine fuel or nitrogen tetroxide oxidizer were developed in the early 1960s by the Air Force Cambridge Research Laboratory. At this time, the type of release anticipated by the Air Force at these sites was a single propellant spill, and the predictions of the toxic vapor corridors upon release into the atmosphere were based on the evaporation of the single propellant and on its subsequent dispersion. The techniques developed by the Air Force Cambridge Research Laboratory to determine these toxic corridors were incorporated into the operational procedures when the Titan II was deployed.

In 1980, a Titan II accident occurred near Damascus, Arkansas in which the scenario was much different than the one for which the toxic hazard corridor calculation procedures were developed. Leaking fuel within the silo eventually made contact with the oxidizer on board a Titan II, leading to a violent explosion which sent combustion products and possibly some unreacted propellant several thousand feet in to the air, where the atmospheric dispersion process began. This effort is designed to characterize the interactions of hypergolic liquid rocket propellants and to provide

information pertinent to the development of a model which would describe the transport and diffusion process of the airborne combustion products and unreacted propellant vapors resulting from a catastrophic accident involving hypergolic liquid rocket propellants.

SECTION II

COMPILATION OF BACKGROUND INFORMATION

Information with respect to hypergolic interactions between hydrazine fuels and nitrogen tetroxide oxidizers was obtained from a variety of sources. The Air Force Project Officer supplied several literature references which were invaluable in determining critical fireball parameters such as fireball size, duration, and thermal energy. Technical reports, documents, and literature sources relative to the identification of combustion products, fireball generation, and chemical reaction kinetics in the reaction between the hypergolic liquid rocket fuels were identified through a NASA-RECON and a Chemical Abstracts computer search.

Past experiments involving reactions between hydrazine fuels and nitrogen tetroxide/nitrogen dioxide oxidizers have been identified in the literature reference articles, including the analysis of the Project Pyro tests. The results of these experiments have identified vapor phase and condensed phase reaction products resulting from the mixing of two hypergols and have generated representative explosive yield characteristics for the hypergolic reaction. In addition to the established combustion products of aerozine-50 with nitrogen tetroxide (which include nitrogen, carbon dioxide, and water vapor), approximately 60 additional chemical species resulting from this hypergolic fuel-oxidizer combustion have been reported in the literature. While the identification and quantification of all such chemical reaction products is too exhaustive and detailed for the present task, some of these chemical species may be important components in the combustion fireball due to thermal or toxicity considerations. Dimethylnitrosamine (NDMA), for example, is an expected and confirmed product from the nitrogen tetroxide - diemthyl hydrazine reaction[1] and also is a known carcinogen.

Information from past accidents which involved reactions of hypergolic rocket propellants has also been evaluated with respect to the thermophysical analysis pertinent to the present effort. Results from the Atlas/Centaur Launch Hazards Assessment Program and the Titan II accident in 1980 were included in this evaluation.

SECTION III

THE CHEMISTRY OF THE HYDRAZINE/NITROGEN TETROXIDE BIPROPELLANT SYSTEM

The hypergolic combination of hydrazine-type fuels (including hydrazine, monomethylhydrazine [MMH], 1, 1 - dimethlyhydrazine [UDMH], and aerozine-50 (A-50, a 50:50 mixture of hydrazine and UDMH by weight) with nitrogen tetroxide [NTO] oxidizers are used in current propulsion systems such as the Titan II Weapons System and the Shuttle Transportation System. This is of the high specific impulse imparted to the launch vehicle by the chemical energy released upon mixing the hypergols in the rocket engine.

The stoichiometric reaction between aerozine-50 and nitrogen tetroxide (the bipropellant system used in the Titan II Weapons System) may be represented by the following equation[2]:

$$.6522\ N_2H_4 + .3478\ C_2H_8N_2 + \frac{O/F}{2.245}\ (1.0217)\ N_2O_4 \longrightarrow \text{Products} \qquad (1)$$

where O/F is the oxidant-fuel mass ratio (2.245 for stoichiometric combustion) and the products of combustion consist primarily of water vapor (H_2O), nitrogen gas (N_2), carbon monoxide (CO), carbon dioxide (CO_2), hydrogen gas (H_2), and hydroxide radical (OH). The available chemical energy from reacting one gram mole of aerozine-50 (.6522 mole hydrazine + .3478 mole UDMH) with 1.02 moles of nitrogen tetroxide at 25°C (298°K) is approximately 1.54×10^5 calories (6.63×10^3 BTU per pound aerozine-50 reacted). This value was calculated from the standard heats of formation of chemical reactants and gaseous reaction products for the stoichiometric hypergolic reaction referenced at 298°K, and will be discussed in more detail in Section IV.

In addition to the formation of the gaseous combustion products described above for a stoichiometric reaction between aerozine-50 fuel and nitrogen tetroxide oxidizer, several competing side reactions occur upon mixing of the two hypergols, and over 50 chemical species have been isolated and identified either as chemical intermediates or condensed phase reaction products in the A-50/NTO hypergolic reaction.

A list of reported secondary chemical reaction products that result from the interaction of Aerozine-50 fuel and nitrogen tetroxide oxidizer is included in Table I. Some of these side products (such as hydrazine nitrate and hydrogen azide) have been identified as the reaction condensates responsible for the "hard start" and "popping" phenomena characteristic of hydrazine-NTO pulsed rocket engines[3,4,5]. While these particular chemical residues affect engine performance and ignition threshold, the instability of these compounds at elevated temperatures suggests their absence in a hypergolic fireball resulting from a propellant accident during transportation or handling. The hydrazine nitrates and azides; therefore, are not seen to be airborne toxins in an accidental hypergolic explosion. Other chemical reaction products are more stable, especially at lower temperatures ($500^{o}K$), and the presence of these compounds in a hypergolic fireball may significantly impact the toxic vapor corridors for a bipropellant accident scenario. The chemical species in this category include dimethylnitrosamine (NDMA), methyl amine, dimethyl amine, formaldehyde, hydrogen cyanide, ammonia, and formaldehyde dimethylhydrazone (FDH). In addition to these reaction products, unreacted propellant vapors (hydrazine vapor, UDMH vapor, nitrogen dioxide) resulting from incomplete combustion and volatilization of excess propellant will also pose a health hazard upon atmospheric dispersion, since both the hydrazine fuel and nitrogen tetroxide oxidizer are extremely toxic, in both the liquid and vapor states.

Most of the reaction products cited in the literature and listed in Table I can be accounted for by one or more of the following chemical reaction mechanisms.

TABLE I

REACTION PRODUCTS IDENTIFIED IN THE AEROZINE-50
NITROGEN TETROXIDE REACTION

No.	Compound Name	Molecular Formula	Reference
1	nitrogen	N_2	1,3,6
2	hydrogen	H_2	3,6
3	water	H_2O	3,6
4	oxygen	O_2	3,6
5	carbon dioxide	CO_2	1,3
6	carbon monoxide	CO	1,3
7	ammonia	NH_3	1,3,6
8	nitrogen dioxide	NO_2	1,3
9	nitrous oxide	N_2O	3,6
10	nitric oxide	NO	3,6
11	hydroxide	OH	2
12	monatomic hydrogen	H	2
13	monatomic oxygen	O	2
14	nitrogen trioxide	N_2O_3	2
15	nitric acid	HNO_3	3,6
16	nitrous acid	HNO_2	3,6
17	hydrogen azide	HN_3	3
18	hydrazine azide	$N_2H_5N_3$	3,5
19	methanol	CH_3OH	1,3
20	methyl amine	CH_3NH_2	1
21	dimethyl amine	$(CH_3)_2NH_2$	1

TABLE I (Continued)

REACTION PRODUCTS IDENTIFIED IN THE AEROZINE-50
NITROGEN TETROXIDE REACTION

No.	Compound Name	Molecular Formula	Reference
22	formamide	CNH_2O	1
23	formaldehyde	CH_2O	3
24	nitrosamine	NH_2NO	3,6
25	dimethylnitrosamine	$(CH_3)_2NNO$	1,3
26	dimethylformamide	$(CH_3)_2NCO$	1
27	methylnitrosamine	HCH_3NNO	1
28	hydrazine nitrate	$N_2H_5NO_3$	1,3,4,7
29	hydrazine dinitrate	$N_2H_4 2HNO_3$	3,5
30	hydrazine nitrite	$N_2H_5NO_2$	3,5
31	dimethylhydrazine nitrate	$(CH_3)_2NH_3NO_3$	1,3
32	ammonium nitrate	NH_4NO_3	3,6
33	ammonium azide	NH_4N_3	3
34	ammonium nitrite	NH_4NO_2	3
35	formaldehyde dimethylhydrazone	$CH_2NN(CH_3)_2$	3
36	tetramethyl tetrazine	$(CH_3)_4N_4$	3
37	tetrazine	H_4N_4	3
38	formaldehyde monomethylhydrazone	CH_2NNHCH_3	3
39	triazine	H_3N_3	3
40	azine	H_2NNNH	3
41	monomethylhydrazine	CH_3HNNH_2	3
42	methyl azide	CH_3N_3	3

TABLE I (Concluded)

REACTION PRODUCTS IDENTIFIED IN THE AEROZINE-50
NITROGEN TETROXIDE REACTION

No.	Compound Name	Molecular Formula	Reference
43	nitromethane	CH_3NO_2	3
44	methyl ammonium nitrate	$CH_3NH_3NO_3$	3
45	nitrosohydrazine	N_2H_3NO	3
46	diazomethane	CH_2N_2	3
47	tetramethylhydrazine	$(CH_3)_4N_2$	8
48	methyl nitrite	CH_3NO_2	3
49	methane	CH_4	3
50	ethane	C_2H_6	3
51	propane	C_3H_8	3
52	acetylene	C_2H_2	3
53	hydrogen cyanide	HCN	3
54	formic acid	HCOOH	3
55	cyanic acid	HOCN	3
56	butadiene	C_4H_6	3
57	ethyl azide	$C_2H_5N_3$	3
58	ethylene	C_2H_4	3
59	nitrilohydrazine	CNN_2H_5	3

A. FREE RADICAL REACTION

The oxidant, N_2O_4, or more precisely the monomer NO_2 is a molecule with an unpaired electron and is thus capable of forming free radicals. The NO_2 free radical can dimerize, add to double bonds, abstract hydrogen, and "activate" other chemical species for further chemical reactions. Figure 1 details a reaction mechanism between hydrazine type fuels and nitrogen tetroxide oxidizer through a NO_2-free radical intermediate.

For the hydrazine reactant A (R = H, R' = H), the intermediate products are ammonia (E), nitrosamine (F) and ammoniun nitrate (G).

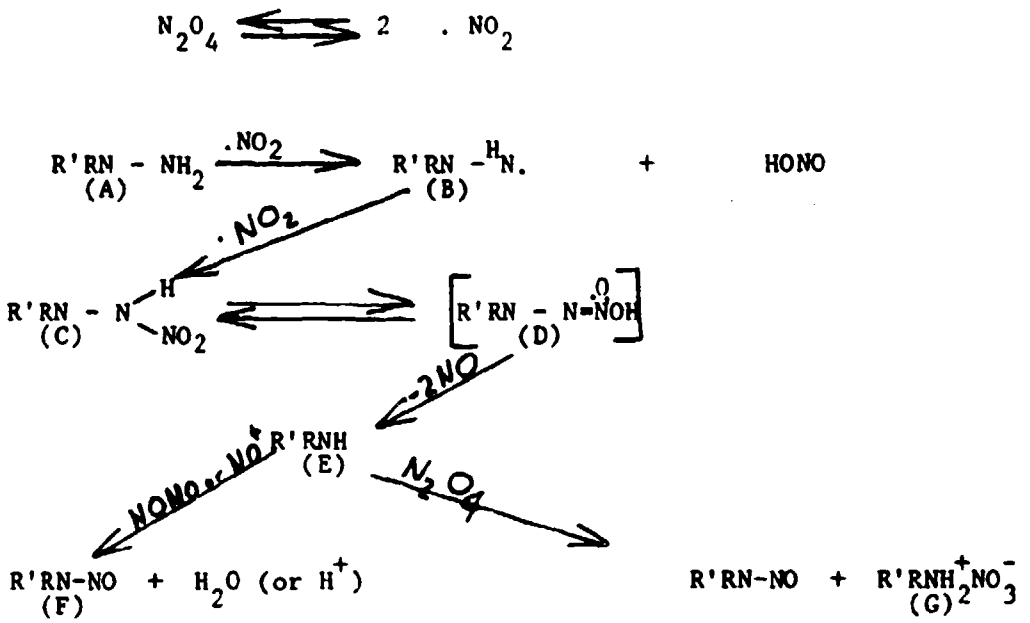
For the monomethyl hydrazine reactant A (R = H, R' = CH_3) the intermediate products are monomethyl amine (E), methylnitrosamine (F), and methyl ammonium nitrate (G).

For the 1, 1-dimethylhydrazine reactant A (R = CH_3, R' = CH_3), the intermediate products are dimethyl amine (E), dimethylnitrosamine (F), and dimethyl ammonium nitrate (G).

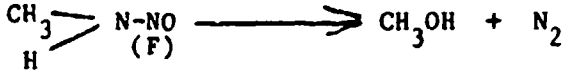
Note that only dimethylnitrosamine is stable upon the oxidation by N_2O_4. Nitrosamine readily decomposes to water and nitrogen, and monomethylnitrosamine decomposes to methanol and nitrogen.

B. NITROSATION REACTION

Figure 2 shows a postulated mechanism and reaction products resulting from the nitrosation of hydrazines by nitrosonium ion (NO^+), formed from the ionization of nitrogen tetroxide which is promoted by donor solvents such as amines and hydrazines.



if R' = CH_3 and R = H, then



if R = R' = H, then

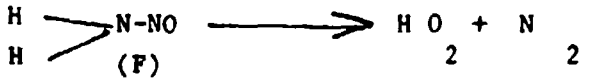


Figure 1. Proposed Free Radical Mechanism for Reaction of N_2O_4 with Hydrazine (Reproduced from Reference 1)

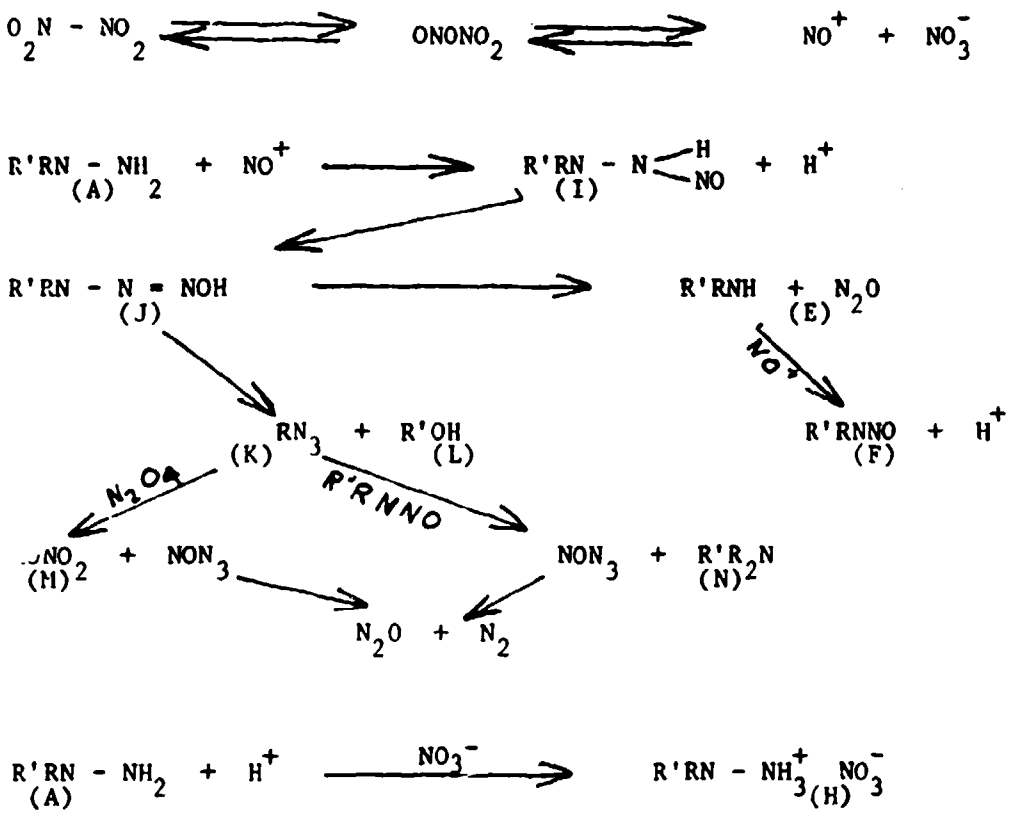


Figure 2. Proposed Nitrosation Mechanism for Reaction of N_2O_4 with Hydrazines (Reproduced from Reference 1)

This reaction also accounts for the formation of substituted amines (products E + N), nitrosamines (product F) and methanol or water (product L). It also indicates the formation of nitrosohydrazine (product I), the azides (methyl and hydrogen, product K) and methyl nitrate or nitric acid (product M). The substituted hydrazinium nitrates (product H) are formed from the reaction of substituted hydrazines with nitric acid.

Several of these species may also form via a simpler mechanism. Since water is a reaction product of the hydrazine/nitrogen tetroxide reaction, the water generated by this hypergolic reaction may react with unreacted nitrogen tetroxide to form nitrous acid and nitric acid, which may subsequently react with the substituted hydrazines to form azides, nitrosamines, and hydrazinium nitrates.

$$R'RN - NH_2 + N_2O_4 \longrightarrow CO_2 + H_2O + N_2 + \text{other products} \quad (2)$$

$$N_2O_4 \rightleftharpoons 2NO_2 \overset{H_2O}{\rightleftharpoons} HNO_2 + HNO_3 \quad (3)$$

$$\underset{(A)}{R'RN - NH_2} + HNO_2 \longrightarrow \underset{(F)}{R'RNNO} + \underset{(E)}{RR'NH} + N_2O + H_2O \quad (4)$$

for R' = R - H,

$$H_2N - NH_3 + HNO_2 \longrightarrow HN_3 + H_2O + H^+ \quad (5)$$

$$\underset{(A)}{R'RN - NH_2} + HNO_3 \longrightarrow \underset{(H)}{R'RN - NH_2 - NO_3^+ \; NO_3^-} \quad (6)$$

The occurrence of the other reaction products in the aerozine-50/nitrogen tetroxide reaction can be best explained by the oxidation of methanol by NO_2 (or N_2O_4) which produces formaldehyde. The formaldehyde can further react to form acetic acid, formamide or an N-substituted formamide, formic acid, and formaldehyde dimethyl hydrazone[1].

In general, the appearance and relative composition of the reaction products described above depend on the oxidizer/fuel ratio, reaction temperature, reaction pressure, degree of mixing of oxidizer and fuel, and geometric and temporal mixing conditions (such as surface area and wall effects, as well as propellant addition rates). As will be subsequently described, few of these secondary reaction products are predicted by chemical equilibrium considerations; most products identified in a reaction mixture therefore are frozen in a nonequilibrium state due to kinetic barriers. Since activation energies for the various reaction pathways are not readily available, prediction of the absolute amounts of these secondary products in a given hypergolic reaction is difficult at best.

C. ATMOSPHERIC OXIDATION OF HYPERGOLIC ROCKET FUELS

Hypergolic liquid rocket fuel (hydrazine, MMH, UDMH) will react with atmospheric oxygen to produce some of the same oxidation products identified in the fuel/nitrogen tetroxide reactions. Because oxygen is a weaker oxidizer than NTO, the stable oxidation products resulting from the interaction of the hydrazine fuels with air are intermediates in the hydrazine/NTO reaction. For example, formaldehyde dimethyl hydrazone (FDH) has been identified as a minor oxidation product or intermediate in the UDMH/NTO reaction but as the major oxidation product in the UDMH/air reaction. These air oxidation products are important in catastrophic accidents in which unreacted liquid fuel or fuel vapors are exposed to the air, particularly upon atmospheric dispersion of unreacted fuel vapors.

1. Hydrazine Autoxidation

Hydrazine reacts with atmospheric oxygen to produce nitrogen and water according to Equation (7).

$$N_2H_4 + O_2 \longrightarrow N_2 + 2H_2O \qquad (7)$$

A side product of this air oxidation of hydrazine vapor is gaseous ammonia, and the rate of the main reaction, as well as the side reaction producing ammonia has been determined to be strongly dependent on surface area and geometric factors[9].

Hydrazine may also decompose in the absence of air to form ammonia, nitrogen, and hydrogen according to several pathways, the most generally accepted on is represented in Equation (9).

$$N_2H_4 \longrightarrow NH_3 + 1/2\ N_2 + 1/2\ H_2 \qquad (9)$$

This reaction, often termed hydrazine monodecomposition, occurs only in the presence of an appropriate catalyst (e.g., metal surfaces) or upon sparking or detonation of vapor mixtures[6,10]. Thus, unreacted hydrazine vapors may be expected to form ammonia, nitrogen, and hydrogen gas with the release of thermal energy under conditions in which the accidental mixing of hypergolic rocket fuels favors a detonation reaction or explosion.

2. Oxidation of Substituted Hydrazines

The major oxidation products identified in the MMH/air reaction are formaldehyde monomethyl hydrazone (FMH), methane, methanol, nitrogen, and water[11]. The reaction between UDMH and air produces FDH, nitrogen, and water according to the stoichiometry in Equation (10).

$$3\ (CH_3)_2NNH_2 + 2O_2 \longrightarrow 2(CH_3)_2NNCH_2 + N_2 + 4H_2O \qquad (10)$$

Diazomethane, dimethylamine, ammonia, and NDMA have been identified as minor products in the UDMH/air reaction[11].

D. ATMOSPHERIC REACTIONS OF HYPERGOLIC ROCKET OXIDIZERS

Unreacted liquid rocket oxidizer (NTO) may vaporize during an accident involving hypergolic rocket propellants to product nitrogen tetroxide vapors and nitrogen dioxide vapors. The proportion of nitrogen tetroxide to nitrogen dioxide in the vapor phase is controlled by the equilibrium constant K_p for the reaction:

$$2\ NO_2 \overset{K_p}{\rightleftharpoons} N_2O_4 \qquad K_p = \frac{p\ N_2O_4}{(p\ NO_2)^2} \tag{11}$$

Where $p\ N_2O_4$ = partial pressure N_2O_4 vapor at equilibrium
$p\ NO_2$ = partial pressure NO_2 vapor at equilibrium

The equilibrium constant K_p for the association of two molecules of nitrogen dioxide gas into one molecule of nitrogen tetroxide gas is temperature-dependent and can be calculated by the Gibbs free-energy function for the association reaction [Equation (11)]:

$$\Delta G^o = -RT \ln K_p = -13600 + 412.6\ T \tag{12}$$

Where R = gas constant (1.987 $^{cal}/_{mole} = {}^oK$)
K_p = association equilibrium constant (1/atm)
T = gas temperature (^oK)
ΔG^o = Gibbs free energy (calories/mole)

The equilibrium mole fractions of nitrogen tetroxide gas and nitrogen dioxide gas as a function of temperature as calculated from Equations (11) and (12) are presented in Table II. In this case, the mole fractions of nitrogen

oxide vapors (NO_2 or N_2O_4) are equal to the partial pressures of the vapors at one atmosphere total pressure. The percent of dissociation of nitrogen tetroxide dimer to nitrogen dioxide monomer, as defined in Equation (13), is also presented in Table II. Thus, above 100°C (373°K), unreacted nitrogen tetroxide gas is virtually completely dissociated into nitrogen dioxide gas[12].

$$\text{Percent Dissociation} = \frac{p\ NO_2 \quad X \quad 100}{p\ NO_2 + 2p\ N_2O_4} \qquad (13)$$

TABLE II. EQUILIBRIUM COMPOSITION OF NITROGEN TETROXIDE AND NITROGEN DIOXIDE IN THE VAPOR PHASE AS A FUNCTION OF ABSOLUTE TEMPERATURE

(P_{Total} = 1 Atmosphere)

Temperature °K	Mole Fraction N_2O_4	Mole Fraction NO_2	Percent Dissociation
298	.698	.302	18
313	.539	.461	30
323	.426	.574	40
373	.066	.934	88

Oxidizer vapors evolved during a hypergolic propellant accident, which will include both N_2O_4 and NO_2 gases, will react with the atmospheric components of air during fireball generation and aerial dispersion. These vapors are expected to react with molecular oxygen to produce a mixture of nitrogen oxides (NO_x) which may include nitrogen trioxide (NO_3; x = 3), dinitrogen trioxide (N_2O_3; x = 3/2) and dinitrogen pentoxide (N_2O_5; x = 5/2). They will also react with atmospheric water vapor to produce both nitrous acid (HNO_2) and nitric acid (HNO_3). The latter phenomenon is known as the acid rain effect. Vaporized rocket oxidizer may also react with any hydrocarbon pollutants in the atmosphere, and these interactions are detailed in Reference 13.

SECTION IV

THERMOCHEMICAL ANALYSIS OF A HYPERGOLIC REACTION

Upon mixing of the hypergolic rocket propellant (A-50 and NTO) during an accidental spill or missile tank rupture, the chemical energy of the propellants is converted into thermal energy used to heat the hypergolic combustion products, to vaporize excess unreacted propellant, and to heat the surroundings in the vicinity of the accident. The thermal energy of the resultant fireball, as well as a measure of the time-dependent energy release of the fireball (heat flux) upon fireball generation and lift-off, are important in the quantification of the release height of the chemical components contained in the fireball and the subsequent deposition pattern upon aerial dispersion.

Thermochemical analysis for hypergolic fireballs were calculated for three separate cases: (1) Fireball combustion products were identified and adiabatic flame temperatures were calculated, using theoretical thermodynamic combustion properties of the hypergolic propellants and the gaseous reaction products; (2) Where the oxidizer to fuel ratio was far removed from stoichiometric combustion, the chemical reaction was treated as a nonequilibrium condition, in which the resultant thermal energy of the fireball was used to heat and vaporize the excess propellant; and (3) The time - temperature profile of a hypergolic fireball was calculated, assuming radiative heat transfer to the environment. These analyses, as well as the determination of the fireball size, are detailed in the sections that follow.

A. ADIABATIC FLAME TEMPERATURE AND CHEMICAL COMPOSITION CALCULATED UNDER EQUILIBRIUM CONDITIONS

Quantification of equilibrium chemical species and calculation of fireball adiabatic temperatures resulting from stoichiometric and nonstoichiometric

reactions of aerozine-50 with nitrogen tetroxide were accomplished using a computer program to calculate complex chemical equilibrium composition (NASA SP-273)[14]. The program solves equations by reiteration to minimize the Gibbs free energy of the chemical reaction products and maintain a mass balance between the chemical reactants (hypergolic propellants) and chemical products (combustion products, oxidation products, and unreacted propellants). This particular program has been routinely used at Martin Marietta to calculate rocket performance parameters for Titan launch vehicles employing hypergolic propellants. The program employs approximately 60 possible reaction products resulting from a particular hypergolic propellant combination.

Flame temperatures of hypergolic fireballs were calculated by this program for an adiabatic condition, i.e., conductive, convective, and radiative heat losses to the environment are negligible. In this case, the heat of reaction of combining (a) moles of A-50 with (b) moles of NTO at 25°C (298°K) was used to heat the resultant chemical species in the fireball from 25°C to the final flame temperature T_F.

For the hypergolic chemical reaction:

$$a\ C_{.696}H_{5.39}\ N_2 + bN_2O_4 \longrightarrow \sum_J n_j P_j + \Delta H_{reaction} \qquad (14)$$

where:

a = number of moles of A-50 reacted

b = number of moles of NTO reacted

n_j = number of moles of combustion product P_j

$\Delta H_{reaction}$ = heat evolved from chemical reaction (calories/mole or BTU/pound)

The adiabatic flame temperature (T_F) is calculated for the hypergolic reaction as follows:

$$\Delta H_{reaction} = a\Delta H_f^o\ (A\text{-}50) + b\Delta H_f^o\ (NTO) - \sum_j n_j \quad \Delta H_f^o\ (P_j)$$

$$= \int_{298}^{T_F} n_j\ C_{pj} dT \qquad (15)$$

For unreacted propellant vapors (P_K) which may be hydrazine vapor, UDMH vapor, NTO vapor or NO_2 vapor depending on the relative amounts of fuel and oxidizer involved in the hypergolic accident (O/F mole ratio is 1.02 for stoichiometric combustion), the enthalpy change from 298°K to T_F includes a phase transition, therefore the final thermochemical equation which includes both gaseous combustion products and vaporized propellant may be written

$$(a + a_1)\ \Delta H_f^o\ (A\text{-}50) + (b + b_1)\ \Delta H_f^o\ (NTO) - \sum_j n_j\ \Delta H_f^o\ (P_j)$$

$$= \int_{298}^{T_F} n_j\ C_{pj}\ dT + \int_{298}^{T_v} n_k\ C_{pk}\ dT + \sum_k n_k\ \Delta H_{vap}\ (P_k)$$

$$+ \int_{T_v}^{T_F} n_k\ C_{pk}\ dT \qquad (16)$$

Where:

a_1 = number moles excess A-50 vaporized

b_1 = number moles excess NTO vaporized

ΔH_f^o = the standard heat of formation of the liquid rocket propellants (A-50 or NTO); or the standard heat of formation of the j^{th} gaseous combustion product

C_{pj} = the constant pressure heat capacity for the j^{th} gaseous combustion product

n_k = the number of moles of k^{th} unreacted vaporized propellant

C_{pk} = the constant pressure heat capacity for the k_{th} unreacted propellant at the temperature interval of interest

T_v = temperature (^oK) at phase transition

ΔH_{vap} = latent heat of vaporization at T_V ^oK

Computer calculations were performed for oxidizer-to-fuel (O/F) mole ratios between 0.0102 and 510.0. The O/F mole ratio for stoichiometric combustion is 1.02, and the O/F mole ratio for the full inventory of hypergolic propellant contained in the Titan II missile (104,609 pounds aerozine-50 and 207,560 pounds nitrogen tetroxide) is approximately 0.90. The calculations were also performed at several reaction pressures intended to simulate different accident scenarios:

1. Combustion in an Open-Field or Vented Environment

P_1 = 1.0 atm

The hypergolic reaction pressure was defined as 1.0 atmosphere (14.7 psia) for propellant accidents in which the gaseous combustion products were allowed to expand and release in an unconfined space. This analysis would be representative of an open-field propellant spill, or a silo spill in which the blast cover door was removed or vented.

2. Confined Silo Fire with Minimal Explosion Hazard

P_2 = 12.56 atm

This situation is intended to represent a bipropellant accident in a confined Titan II missile silo (700-ton horizontal silo door intact) in which the propellant leak rate is too slow to allow any overpressure conditions in the silo due to deflagration or detonation of the combined hypergolic rocket propellants. In this case, the silo pressure will slowly rise until the 700

ton blast door will be ejected, and the resultant fireball will be subsequently released from the opened silo. The pressure at fireball lift-off time can be calculated from the force required to remove the horizontal silo door as follows:

P_2 = Pressure required to eject silo cover =

$$\frac{\text{Weight Silo Door (Pound) + 4X Shear Force T-Lock Restraint}}{\text{Exposed Surface Area Silo Door}} \qquad (17)$$

$$P_2 = \frac{1.4 \times 10^6 \text{ Lb} + 4(5.5 \times 10^5 \text{ Lb})}{954 \text{ Ft}^2} = 2.45 \times 10^4 \text{ Lb/Ft}^2$$

P_2 = 185 psia = 12.56 atmospheres

3. Open Silo Hypergolic Explosion

$$P_3 = 1.0 \text{ atmosphere} + P_{over}$$

This analysis is performed to estimate a large-scale propellant spill in which the propellants spill out of missile tankage and mix in an open silo. In this case the spill and mixing rates of the hypergolic propellants are large enough to initiate a chemical explosion. Detonation reactions between hydrazine-type fuels and nitrogen tetroxide oxidizer have been previously documented in the literature[15,16]. The analyses for the detonation shock front resulting from the accidental explosion has been calculated, using the geometric conditions present in the Titan II launch tube. The area available for expansion of the shock front in this case is equal to twice the cross-sectional area of the launch tube (expansion in two directions) minus the void cross-sectional area of the missile. This is

$$2(\pi R^2) - 2(\pi R'^2) = 946 \text{ Ft}^2 \qquad (18)$$

where:

R = radius of launch tube = 13 2 Feet

R' = radius of missile = 5 Feet

Many different factors can affect the severity of the shock overpressure[15]. The most significant of these are:

a. Total propellant weight
b. Propellant type
c. TNT equivalent yield
d. Geometry of surroundings.

The relevant geometry for an in-silo explosion resulting from the mixing of the two hypergolic propellants has been defined above.

The TNT equivalent yield is a measure of the explosive potential of the detonation reaction, i.e., the TNT yield is the weight fraction of the explosive substance which is equal to the same weight of TNT. In hypergolic explosions between A-50 fuel and NTO oxidizer, a 0.5 percent TNT equivalent yield conservative maximum can be expected from Project Pyro test data[16].

The static peak overpressure for the detonation blast wave is the measured air pressure in the shock front, and is related to the total propellant weight, TNT equivalent yield and reduced distance (λ) by the following equation:

$$\log P_{over} = -2.349 \log \lambda + 3 \qquad (19)$$

where P_{over} = the static peak overpressure (psig) and λ = the reduced distance.

In theory, a given overpressure will occur at a distance from an explosion proportional to the cube root of the energy yield or to the cube root of the explosive weight. Full-scale tests indicate that this relation between distance and energy released holds for explosive yields into the megaton range:[15]

$$\lambda = \frac{r}{(\%W)^{1/3}} \tag{20}$$

where r = equivalent silo hemisphere radius

$\lambda = (946/2\pi)^{1/2} = 12.3$ Feet

and percent W = Equivalent explosive weight involved in hypergolic reaction (does not include unreacted vaporized propellant),

Equation (19), which was valid for 1000-pound Project Pyro test data for reduced distances (λ) between 1.0 and 10.0, can be combined with Equation (20) to give the final static overpressure equation:

$$\log P_{over} = -2.349 \log \left[\frac{12.3}{(.005\ W_b)^{1/3}} \right] + 3 \tag{21}$$

Where W_b = the total liquid propellant weight (pounds) involved in the hypergolic reaction.

From Equation (21), hypergolic reactions involving large quantities of mixed propellants are more catastrophic in nature, resulting in higher static peak overpressures and explosive detonation. As the total propellant weight involved in the hypergolic reaction (W_b) decreases, the peak overpressure decreases and the accident scenario more closely resembles a nonexplosive chemical combustion.

For an accident involving the full inventory of rocket propellant in a properly fueled Titan II missile (W_b = 3.122 X 10^5 Lb) the equivalent yield is 1.56 X 10^3 Lb TNT, and the calculated peak overpressure is 872 psig (60.3 atmospheres). This pressure was therefore used to calculate the theoretical thermodynamic combustion products and adiabatic flame temperatures resulting from a catastrophic accident involving the full inventory of liquid rocket propellant contained in the Titan II missile (Stage 1 and Stage 2).

4. Confined Silo Hypergolic Explosion

P_4 = 12.56 atmosphere + P_{over}

The situation in which a catastrophic hypergolic accident occurs in a closed missile silo has been approximated by assuming an initial slow pressure buildup followed by an explosive detonation of mixed propellants. In this case, the maximum silo pressure before ejection of the 700-ton horizontal silo door would be the pressure required to eject the silo cover (12.56 atmospheres) plus the static peak overpressure resulting from the hypergolic explosion. For a catastrophic accident involving the mixing of the full propellant load in a sealed Titan II missile silo, the maximum pressure calculated is 12.56 atm + 59.3 atm overpressure = 71.9 atmospheres total pressure. This pressure is considered a worst-case explosive condition. In accidents which involve the accidental mixing of hypergolic propellants in a sealed silo, the actual silo pressure will depend on the rate of propellant mixing, and on the configuration of the missile and silo prior to the accident. For example, peak overpressures would be different for conditions in which Stages I and II are confined in the silo than for those conditions which result in the expulsion of Stage I and/or II, plus the reentry vehicle (RV) from the silo. The latter case was typical of the accident scenario near Damascus, Arkansas. The total pressure in the sealed silo prior to fireball lift-off is therefore bounded by the minimum pressure to eject the silo door (12.56 atm) and the maximum pressure due to a hypergolic explosion (12.56 atm + P_{over}).

Fifteen computer calculations were performed for various hypergolic combinations simulating an in-silo mixing accident (silo door open or closed) or an open-field accident. A description of the computer input pertinent to these 15 calculations is presented in Table III. Results of these 15 computer runs, referenced by their respective case numbers are found in Appendix A. The first five runs are calculated for an O/F mole ratio of .902 (the ratio used in the fueling and firing of a Titan II missile). These calculations were also performed, assuming thermal interaction of the air present in the silo (125,000 Ft^3 air). The total propellant weight was decreased from 3 X 10^5 pound in Run 1 to 3 X 10^2 pound in Run 5, while the O/F mole ratio (.90) and weight of silo air (9,475 pound) were held constant.

TABLE III. INPUT TO SP-273 COMPUTER CALCULATIONS FOR BIPROPELLANT ACCIDENTS

Run No.	Case No.	O/F Mole Ratio	O/F Weight Ratio	Weight A-50 Pounds	Weight NTO Pounds	Weight Air Pounds	P_1 atm	P_2 atm	P_3 atm	P_4 atm
1	1	.902	2.076	1.046×10^5	2.076×10^5	9.475×10^3	1	12.56	60.3	71.9
2	2	.902	2.890	1.046×10^4	2.076×10^4	9.475×10^3	1	12.56	----	----
3	3	.902	11.04	1.046×10^3	2.076×10^3	9.475×10^3	1	12.56	----	----
4	4	.902	92.57	1.046×10^2	2.076×10^2	9.475×10^3	1	12.56	----	----
5	5	.902	907.8	10.46	20.76	9.475×10^3	1	12.56	----	----
6	6	1.02	2.348	9.247×10^4	2.076×10^5	9.475×10^3	1	12.56	59	70.6
7	19	1.02	2.245	9.247×10^4	2.076×10^5	0	1	12.56	----	----
8	32	0.51	1.122	9.247×10^4	1.038×10^5	0	1	-----	----	----
9	20	0.204	4.49×10^{-1}	9.247×10^4	4.152×10^4	0	1	-----	----	----
10	21	0.102	2.25×10^{-1}	9.247×10^4	2.076×10^4	0	1	-----	----	----
11	23	0.010	2.25×10^{-2}	9.247×10^4	2.076×10^3	0	1	-----	----	----
12	33	2.04	4.49	4.623×10^4	2.076×10^5	0	1	-----	----	----
13	26	5.1	1.123×10^1	1.849×10^4	2.076×10^5	0	1	-----	----	----
14	28	51.0	1.123×10^2	1.849×10^3	2.076×10^5	0	1	-----	----	----
15	30	51.0	1.123×10^3	1.849×10^2	2.076×10^5	0	1	-----	----	----

Results for the full inventory of liquid rocket propellant (3×10^5 pounds) indicate adiabatic flame temperatures of 2916°K, 3180°K, 3340°K, and 3357°K for silo pressures of 1 atmosphere, 12.56 atmospheres, 60.3 atmospheres, and 71.9 atmospheres respectively. The major fireball constituents for this reaction were carbon monoxide, carbon dioxide, hydrogen gas, water vapor, nitric oxide, nitrogen gas, hydroxide radical, and oxygen gas, the proportion of which varied according to the reaction (silo) pressure. As the total propellant weight decreased, the thermal energy of the combustion products was used to heat the silo air. Thus in Case 5, which employed a 1/1000 propellant load (3×10^2 pound), the adiabatic flame temperature was reduced to 323°K at 1 atmosphere pressure and also 323°K at 12.56 atmospheres pressure. The exact quantity of silo air which will interact with the hypergolic rocket fuels will depend on the extent of mixing and fireball lift-off time.

Run number 7 (Case 19) details the computer results for a stoichiometric mixing of hypergolic rocket propellants (O/F = 1.02) in the absence of interacting air. The results of this analysis, presented in Figure 3, will be used in thermochemical calculations to be described in subsequent sections. Since no air was allowed to interact with the liquid rocket fuel, the calculated adiabatic flame temperature of 2917°K is independent of the total propellant weight, W_b, as long as the O/F ratio remains constant.

Hypergolic spills which involve an excess of A-50 fuel (Computer Runs 8-11) indicate that the calculated equilibrium chemical species contained in the fireball would be carbon black (C), methane gas (CH_4), hydrogen gas (H_2), and nitrogen gas (N_2).

Spills which involve an excess of NTO oxidizer (Computer Runs 12-15) contain mostly nitrogen gas and oxygen gas as equilibrium fireball components with very small amounts of other chemical species present.

These computer results which involve nonstoichiometric mixing of A-50 fuel and NTO oxidizer are accurate for ideal thermodynamic conditions, i.e., when the Gibbs free energy of the reaction products is minimized. Unfortunately, not all chemical reactions occur naturally and within a reasonable time frame to produce the thermodynamically stable product.

As an allotropic form of carbon, graphite is thermodynamically more stable than a diamond. A diamond, however, does not spontaneously revert to the graphite without extremes of temperature. The difference between the actual chemical composition and the thermodynamically predicted compositions may be attributed to the kinetic barrier or energy of activation for the reaction. Since the nonstoichiometric calculations described above for a mixing of hypergolic fuel and oxidizer do not account for kinetic effects, a more realistic approach to fuel-rich or fuel-lean combustion reactions is presented in the following section.

B. VAPORIZATION OF EXCESS UNREACTED PROPELLANTS CALCULATED UNDER NONEQUILIBRIUM CONDITIONS

Because the NASA SP-273 computer program did not predict propellant vaporization due to kinetic factors, an approach was formulated which allows the vaporization of excess liquid rocket propellant and calculates the final adiabatic flame temperature of the resulting fireball under nonstoichiometric conditions.

In general, the fuel and oxidizer reacted stoichiometrically, according to Equation (1) in Section III, and the thermal energy resulting from this chemical reaction was used to vaporize any excess unreacted propellant. The fireball chemical species for nonstoichiometric conditions, therefore, contained the combustion products calculated for Computer Run 7 (Case 19) and the vaporized excess propellant. Because the chemical thermal energy released from the hypergolic reaction was used to vaporize and heat excess propellant, final adiabatic temperatures were significantly lower than those reported in Section A.

Calculations are provided in this section for the following vaporization conditions:

1. All excess fuel (hydrazine + UDMH) vaporized
2. All excess oxidizer (N_2O_4) vaporized
3. UDMH selective evaporation
4. Hydrazine monodecomposition and UDMH evaporation
5. Oxidizer evaporation and dissociation into NO_2

The exact vaporization condition depends strongly on the nature of the hypergolic accident. Condition 4, for example, would be a more likely result than Condition 1 in cases in which the accident involves an explosion, since the decomposition of hydrazine to ammonia occurs catalytically and rapidly when explosively initiated. Condition 5 is the preferred mechanism for oxidizer

vapor release at temperatures above 373°K (refer to Table II - Section D). UDMH selective evaporation may occur during tank rupture because the vapor pressure of UDMH liquid is significantly higher than hydrazine liquid.

The mathematical development of the thermochemical equation required to predict fireball temperatures and chemical compositions in hypergolic reactions involving an excess of A-50 fuel or NTO oxidizer is presented below:

Define:

a_1 = # moles hydrazine liquid reacted
a_2 = # moles UDMH liquid reacted
a_3 = # moles nitrogen tetroxide liquid reacted
a_4 = # moles carbon monoxide (CO) formed by combustion
a_5 = # moles carbon dioxide (CO_2) formed by combustion
a_6 = # moles hydrogen radical (H) formed by combustion
a_7 = # moles hydrogen gas (H_2) formed by combustion
a_8 = # moles water vapor (H_2O) formed by combustion
a_9 = # moles nitric oxide (NO) formed by combustion
a_{10} = # moles nitrogen gas (N_2) formed by combustion
a_{11} = # moles hydroxide radical (OH) formed by combustion
a_{12} = # moles oxygen gas (O_2) formed by combustion
a_{13} = # moles hydrazine vaporized
a_{14} = # moles UDMH vaporized
$2a_{15}$ = # moles NO_2 formed from a_{15} moles N_2O_4
a_{16} = # moles NH_3 formed from hydrazine decomposition
a_{17} = # moles H_2 formed from hydrazine decomposition
a_{18} = # moles N_2 formed from hydrazine decomposition
a_{19} = # moles N_2O_4 vaporized
α = Oxidizer/Fuel mole ratio
P' = Percent Mixing (Fraction of excess propellant vaporized)
X = moles of excess fuel (A-50)
Y = moles of excess oxidizer (NTO)
f = fraction excess $N_2O_4(g)$ dissociated into $2NO_2(g)$ at temperature T(°K)

For an adiabatic process,

$$\Delta H_f^o \text{ reactants} = \Delta H_f^o \text{ products} + \int_{298}^{T_F} {}^{o}C_p \, dT \text{ (products)}$$

where T_F = adiabatic flame temperature

C_p^o = low pressure heat capacity of products

for $C_p^o = A + BT + CT^2 + DT^3$ $\left\{ \begin{array}{l} C_p^o \text{ in cal/mole } {}^oK \\ T \text{ in } {}^oK \end{array} \right.$

then upon integration: ΔH_f^o reactants =

$$\Delta H_f^o \text{ products} + AT_F + \frac{B}{2} T_F^2 + \frac{C}{3} T_F^3 + \frac{D}{4} T_F^4 + E \qquad (22)$$

where $E = -A(298) - \frac{B}{2}(298)^2 - \frac{C}{3}(298)^3 - \frac{D}{4}(298)^4$

The low-pressure heat capacities for fireball reaction products, as well as the standard free energies of formation for reactants and products, were obtained from a variety of sources[14,17,18] and are presented in Table IV. The vapor-phase heat capacity for UDMH was not readily available in the literature so it was estimated by using Dobratz's Equation[19].

Note that the sensible and latent heats for propellant vaporization are not required in this analysis, since these heats are already included in the heats of formation of the propellant vapors at 298°K (ΔH_f^o for species $^a13$, $^a14$, and $^a19$).

TABLE IV. THERMOCHEMICAL PROPERTIES FOR HYPERGOLIC PROPELLANTS AND REACTION PRODUCTS

Coefficient	Species*	ΔH_f^o	Temp Range °K	A	B 10^2	C 10^5	D 10^9	E 10^{-3}
a_1	$N_2H_4(1)$	12054	-----	-----	-----	-----	-----	-----
a_2	UDMH(1)	12339	-----	-----	-----	-----	-----	-----
a_3	$N_2O_4(1)$	-4676	-----	-----	-----	-----	-----	-----
a_4	CO	-26416	273-3700	6.480	0.1566	-.0239	0	-1.998
a_5	CO_2	-94052	273-3700	6.393	1.0100	-.3405	0	-2.324
a_6	H	52094	1000-5000	4.968	0	0	0	-1.480
a_7, a_{17}	H_2	0	273-3700	6.424	0.1039	-.0078	0	-1.960
a_8	H_2O	-57798	273-3700	6.970	0.3464	-.0484	0	-2.227
a_9	NO	21600	273-3700	6.462	0.2358	-.0770	.0873	-2.024
a_{10}, a_{18}	N_2	0	273-3700	6.529	0.1488	-.0227	0	-2.010
a_{11}	OH	9625	1000-5000	5.785	0.1906	-.0386	.0273	-1.805
a_{12}	O_2	0	273-3700	6.732	0.1505	-.0179	0	-2.071
a_{13}	N_2H_4	22434	1000-5000	10.12	1.85	-.6680	1.119	-3.780
a_{14}	UDMH	20705	0-2000	4.06	6.54	-2.18	0	-3.921
a_{15}	NO_2	7960	273-1500	5.481	1.366	-.842	1.88	-2.170
a_{16}	NH_3	-11040	273-1500	6.586	0.6126	.2366	-1.598	-2.253
a_{19}	N_2O_4	2114	273-1500	7.945	4.46	-2.71	0	-4.109

ΔH_f^o = heat of formation (calories/mole)

$C_p = A + BT + CT^2 + DT^3$ (calories/mole °K)

*Species are gaseous unless otherwise noted by (1).

For example:

$$\Delta H_f^\circ \text{ hydazine vapor } (298^\circ K) = \Delta H_f^\circ \text{ hydrazine liquid } (298) - \Delta H_{vap}^{298} \quad (23)$$

$$\text{and } \Delta H_{vap}^{298} = \Delta H_{vap}^{NBP} + C_p^l (T_B - 298) - C_p^v (T_B - 298) \quad (24)$$

therefore

$$\Delta H_{f\ (298,v)}^\circ = \Delta H_{f\ (298,l)}^\circ + C_p^l (T_B - 298) + \Delta H_{vap}^{NBP} - C_p^v (T_B - 298)$$

where l = liquid phase
v = vapor phase
NBP = normal boiling point
T_B = temperature at boiling

Coefficients for a stoichiometric reaction of A-50 fuel and NTO oxidizer were determined from Equation (1), Section III for the reactants (hydrazine, UDMH, and NTO), and from the computer output for stoichiometric combustion (Figure 3) for the normal combustion products. These coeff ·ts are:

$a_1 = .6522$	$a_2 = .3478$	$a_3 = 1.0217$
$a_4 = .3807$	$a_5 = .3149$	$a_6 = .1755$
$a_7 = .3570$	$a_8 = 2.087$	$a_9 = .0726$
$a_{10} = 1.985$	$a_{11} = .3267$	$a_{12} = .59$

Only the major combustion species were included in this analysis, and oxygen (a_{12}) was used to provide a mass balance for the chemical reaction.

CASE NO 19

	CHEMICAL FORMULA					WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N 2.00000	H 4.00000				.50000	12100.000	L	298.15	0.0000
FUEL	C 2.00000	H 8.00000	N 2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N 2.00000	O 4.00000				1.00000	-4676.000	L	298.15	0.0000

O/F= 2.2450 PERCENT FUEL= 30.8166 EQUIVALENCE RATIO= 1.0017 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2918
H, CAL/G	53.5
S, CAL/(G)(K)	3.0162
M, MOL WT	22.448
(DLV/DLP)T	-1.03828
(DLV/DLT)P	1.8176
CP, CAL/(G)(K)	2.0417
GAMMA (S)	1.1173
CPF, CAL/(G)(K)	.4689
SON VEL,M/SEC	1098.9

MOLE FRACTIONS

CO	.06301
CO2	.05210
H	.02952
HO2	.00001
H2	.05926
H2O	.34523
N3	.01260
N2	.32797
O	.01682
OH	.05366
O2	.03980

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .00005 FOR ALL ASSIGNED CONDITIONS

C(GR)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	C2
C2H	C2H2	C2H3	C2H4	C2N	C2N2	C2H2OH(L)	C2H2OH	C2O	C3
C3O2	C3	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3	H2O2(L)
H2O2	N	NCO	NH	NH2	NH3	NO2	NO3	N2H4	N2H4(L)
N2O	N2O4	N2O4(L)	N2O5	N3	O3				

NOTE WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

Figure 3. Computer Output for Stoichiometric Mixing of A-50 and NTO

The coefficients for unreacted vaporized propellants were determined from the O/F mole ratio (α) and vaporization conditions as follows:

1. Excess Fuel Reactions

Define $\alpha = \frac{1.0217}{1 + X}$

$$X = \frac{1.0217 - \alpha}{\alpha}$$

Case 1. All excess hydrazine and UDMH vaporized

a_{13} = moles hydrazine vaporized =
$\beta(.6522X) = \beta(.6664 - .6522\alpha)/\alpha$

a_{14} = moles UDMH vaporized =
$\beta(.3478X) = \beta(.3553 - .3478\alpha)/\alpha$

$a_{15}, a_{16}, a_{17}, a_{18}, a_{19} = 0$

Case 2. UDMH selective vaporization

$a_{14} = \beta(.3553 - .3478\alpha)/\alpha$

$a_{13}, a_{15}, a_{16}, a_{17}, a_{18}, a_{19} = 0$

Case 3. Hydrazine decomposition and UDMH vaporization

$$N_2H_4 \longrightarrow NH_3 + 1/2N_2 + 1/2H_2$$

$a_{14} = \beta(.3553 - .3478\alpha)/\alpha$
$a_{16} = \beta(.6664 - .6522\alpha)/\alpha$
$a_{17} = \beta(.3332 - .3261\alpha)/\alpha$
$a_{18} = \beta(.3332 - .3261\alpha)/\alpha$
$a_{13}, a_{15}, a_{19} = 0$

2. Excess Oxidant Reactions

Define $\alpha = \frac{1.0217 + y}{1}$

$$y = \alpha - 1.0217$$
$$y = \beta(\alpha - 1.0217)$$

a_{15} = # moles excess N_2H_4 = $\beta(\alpha - 1.0217)$
$2a_{15}$ = # moles vaporized NO_2 = $2\beta f \quad (\alpha - 1.0217)$
a_{19} - # moles vaporized N_2O_4 = $(1-f)\beta(\alpha - 1.0217)$

$a_{13}, a_{14}, a_{16}, a_{17}, a_{18} = 0$

Upon multiplication by known coefficients, integration of the heat capacity function, and collection of terms, the final thermochemical equation for nonstoichiometric hypergolic propellant reactions is:

$$\begin{aligned}
&7375.6 + (a_{13} + a_{16})(12054) + a_{14}(12339) + (a_{15} + a_{19})(-4676) \\
&= -.1595\times10^{5} + 41.49T + 8.007\times10^{-3}T^{2} - 1.063\times10^{-6}T^{3} + 3.807\times10^{-12}T^{4} \\
&+a_{13}(\ .186\times10^{5} + 10.12T + 9.25\times10^{-3}T^{2} - 2.227\times10^{-6}T^{3} + 279.8\times10^{-12}T^{4}) \\
&+a_{14}(\ .186\times10^{5} + 4.06T + 32.7\times10^{-3}T^{2} - 7.267\times10^{-6}T^{3} + 0.0T^{4}\ ) \\
&+2a_{15}(\ .058\times10^{5} + 5.48T + 6.83\times10^{-3}T^{2} - 2.807\times10^{-6}T^{3} + 470\times10^{-12}T^{4}) \\
&+a_{16}(-.133\times10^{5} + 6.59T + 3.06\times10^{-3}T^{2} + .788\times10^{-6}T^{3} + -399.5\times10^{-12}T^{4}) \\
&+a_{17}(-.020\times10^{5} + 6.42T + .52\times10^{-3}T^{2} - .026\times10^{-6}T^{3} + 0.0T^{4}\ ) \\
&+a_{18}(-.020\times10^{5} + 6.53T + .74\times10^{-3}T^{2} - .076\times10^{-6}T^{3} + 0.0T^{4}\ ) \\
&+a_{19}(-.020\times10^{5} + 7.95T + 22.3\times10^{-3}T^{2} - 9.03\times10^{-6}T^{3} + 0.0T^{4}\ )
\end{aligned} \qquad (26)$$

Adiabatic Flame Temperatures and Fireball Compositions were calculated for various O/F ratios, vaporization conditions, and mixing conditions and are presented in Appendix B. Note that when $^{a}13$, $^{a}14$, $^{a}15$, $^{a}16$, $^{a}17$, $^{a}18$, and $^{a}19$ are zero, Equation (26) reduces to a stoichiometric combustion, and yields an adiabatic flame temperature of 2979°K. This temperature is approximately 2 percent higher than that predicted by the NASA SP-273 program because not all the combustion products were considered in this analysis and because the heat capacity data used in this analysis were different than the data used in the computer program.

For a fourfold excess of A-50 fuel (O/F = .204, Analysis 5) the adiabatic flame temperature drops to 1046°K, and the mole fractions of hydrazine vapor and UDMH vapor contained in the fireball are 0.25 and 0.14, respectively. The balance of the chemical constituents in the fireball include primarily water vapor (mole fraction .20) nitrogen gas (mole fraction .19), and oxygen (mole fraction .06); with trace amounts of the remaining combustion products. When calculated for hydrazine decomposition with the same fourfold excess of fuel (O/F = .204, Analysis 6), the calculated fireball temperature is 1523°K (increase in temperature due to thermal stability of ammonia vapor over hydrazine vapor) and the major fireball species are hydrogen gas, water vapor, nitrogen gas, UDMH vapor, and ammonia gas.

For a fourfold excess of NTO oxidizer (O/F = 5.1, Analysis 15), the final calculated adiabatic fireball temperature is 810°K and the fireball composition consists primarily of NO_2 gas (mole fraction .57), nitrogen gas (mole fraction .14) and water vapor (mole fraction .14).

The fireball temperature for the oxidizer-rich reaction is much lower than for the fuel-rich reaction, because energy is required to vaporize excess N_2O_4 liquid (ΔH_{vap} N_2O_4 = 6790 cal/mole NTO) and to dissociate the vaporized N_2O_4 molecules into two molecules of nitrogen dioxide gas (ΔH_{diss} N_2O_4 = 13,600 cal/mole NTO). As described previously, both of these heats are accounted for in the standard heat of formation of NO_2 gas at 298°K (coefficient $^{a}15$ in Table IV).

Note that excess propellant vaporization is not predicted for oxidizer/fuel ratios larger than 17.7 or smaller than .06 in cases in which both propellant species are 100 percent mixed. In these cases, the heat of reaction is sufficient to raise the excess propellant liquid temperature (sensible heat) but not sufficient to vaporize the excess propellant (heat of vaporization).

C. CALCULATION OF FIREBALL SIZE AND QUANTIFICATION OF HEAT FLUX

The fireball size and heat flux calculations presented here are based on the mathematical description presented by Sandia Laboratories.[7] This free-field model uses black-body radiation heat losses and continuous expansion of the fireball volume. The convective heat losses and mixing of the reactants and products with the environment are considered negligible during the formation and initial lift-off of the fireball.

1. Theory

The calculations for the fireball formation, using this Sandia Laboratories model, represent the reaction time, t_b, based on a spherical fireball and a hydrodynamic flow model as

$$t_b = 0.6 \quad W_b^{1/6} \tag{27}$$

The reaction time is the time necessary for the mass of hypergolic propellant, W_b, to mix and react to completion. The reaction time, t_b, is also equivalent to the fireball lift-off time. The radius of the fireball, r_b, was determined from the spherical gas volume and the average gas density, $\rho = P\,(MW)/R'T$,

as

$$r_b = (3/4\,\pi\,\rho\,)^{1/3} \quad W_b{}^{1/3} \tag{28}$$

The fireball growth ratio was based on the assumption that the propellant was consumed at a constant rate, R, where

$$R = W/t = W_b/t_b = W_b/(0.6\ W_b^{1/6}) = 5W_b^{5/6}/3. \quad (29)$$

The radius of the fireball as a function of time, t, was determined, using Equation (29) to specify the propellant weight and the methodology used to develop Equation (28). This leads to

$$r = (3\ Rt/4\pi\rho)^{1/3} = C\ t^{1/3} \quad (30)$$

during the time when the propellants are reacting and

$$r = (3W_b/4\pi\rho)^{1/3}\ t^{1/3}$$

after the reaction has terminated and the fireball has lifted off.

The fireball temperature and rate of energy release were determined from an energy balance that equated the enthalpy of the input propellant minus the energy radiated to the environment to the rate of change of internal energy in the fireball. This can be written as

$$Rh_i - \epsilon\sigma\ AT^4 = d\ (Wh)_{fb}/dt \quad (31)$$

for the period of time when propellant is being consumed by the reaction and

$$d\ (Wh)_{fb}/dt = -\epsilon\sigma\ AT^4 \quad (32)$$

after the reaction is complete.

Equation (31) can be rearranged and simplified using the assumptions and definitions outlined above to give the following nonlinear differential equation that was solved numerically for the temperature during the reaction time ($t' \leq 1$):

$$\frac{dT}{dt'} = \frac{h_i - h_{fb} - \frac{4\pi\epsilon\sigma}{1.66 W_b} 1/6 \left[\frac{3t' \quad R'}{4\pi P \quad (M.)}\right]^{2/3} T^{14/3}}{t' C_p} \tag{33}$$

h_i = H_o reactants, enthalpy of reactants

h_{fb} = $\left[H_o + \int C_p dT\right]$ products, enthalpy of products

ϵ = 1 (black body radiation)

σ = Boltzmann's constant

W_b = weight of propellant

t' = t/t_b = nondimensional time

R' = international gas constant

P = 1 atmosphere, pressure of ambient fireball

(MW) = molecular weight of gaseous products

C_p = $A + B\,T + C\,T^2 + D\,T^3$, specific heat of products

T = absolute temperature

Equation (32) can also be rearranged to solved for the temperature of the fireball after the reduction is completed and the fireball lifts off ($t' \geq 1$).

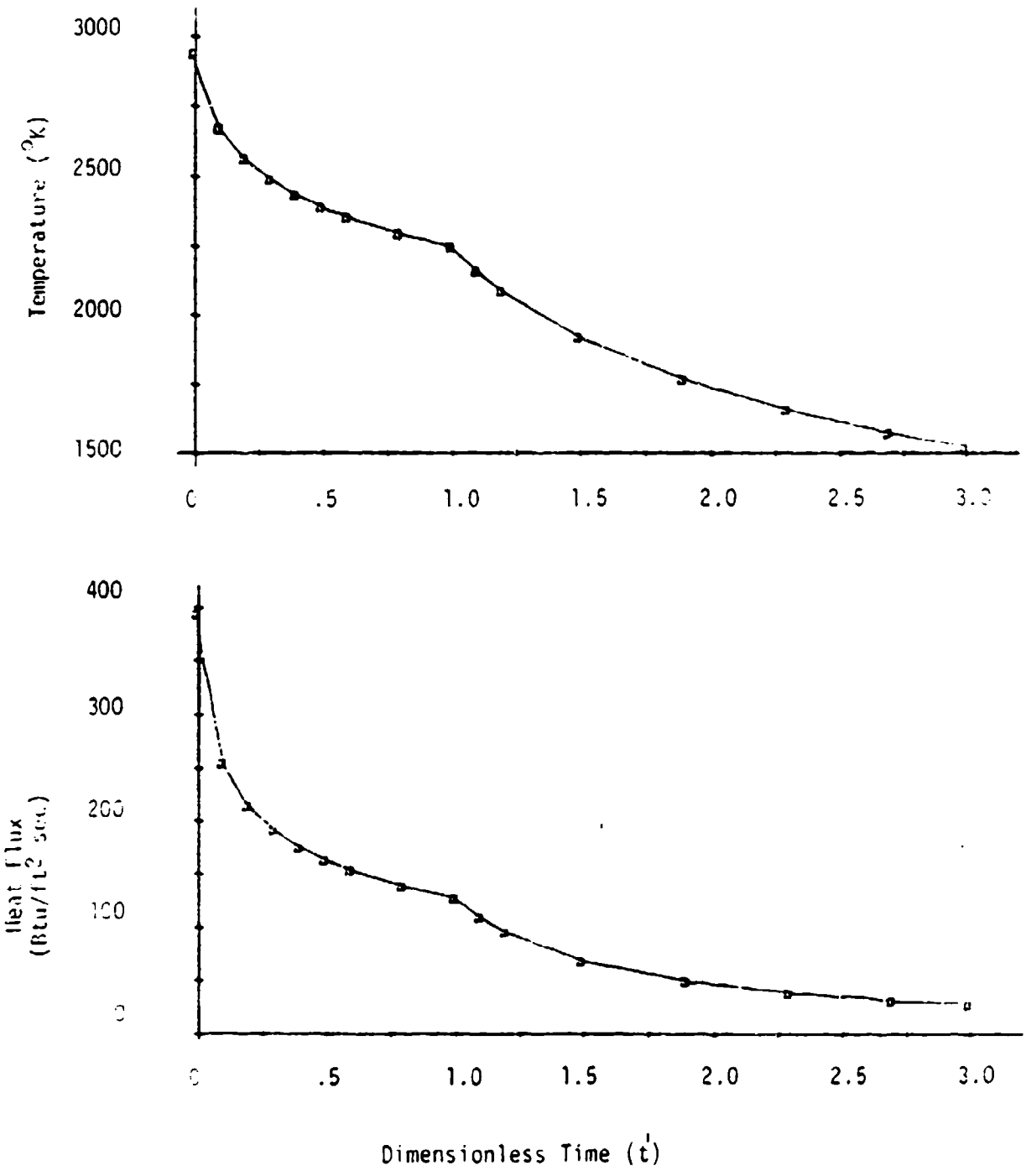
$$\frac{dT}{dt'} = -\frac{4\pi\epsilon\sigma}{1.66 W_b^{1/6} C_p} \left[\frac{3 R'}{4\pi P \quad (MW)}\right]^{2/3} T^{14/3} \tag{34}$$

2. Results

Equations (33) and (34) were integrated numerically, using a Fourth Order Runge - Kutta Method. The initial temperature, $T(t') = T(0)$, for the case during the propellant reaction, Equation (33), is the adiabatic flame temperature. The initial condition for Equation (34) which describes the fireball temperature after lift-off, $t' > 1$, was considered to be the solution of Equation (32) at $t' = 1$.

Figure 4 shows the temperature, dimensionless time relationship for $3X10^5$ pounds of stoichiometric mixture of N_2O_4 and A-50. The initial temperature of the fireball was calculated to be 2979^oK and decreased to 2243^oK at $t' = 1$ which is 4.9 seconds after ignition. The temperature of the rising fireball was calculated to decrease to 1518^oK at $t' = 3$ or $t = 14.7$ seconds after ignition.

Figure 5 shows the radiant heat flux from the fireball as function of t' for this stoichiometric mixture. The initial value is 393 Btu/Sec ft^2 and decreased to 126 Btu/sec ft^2 at $t' = 1$ after the lift-off, $t' > 1$, the heat flux continues to drop off to approximately 27 Btu/sec ft^2 at $t' = 3$.



Figures 4 and 5. Radiative Fireball Temperature and Heat Loss

$W_b = 3.00 \times 10^5$ Pounds

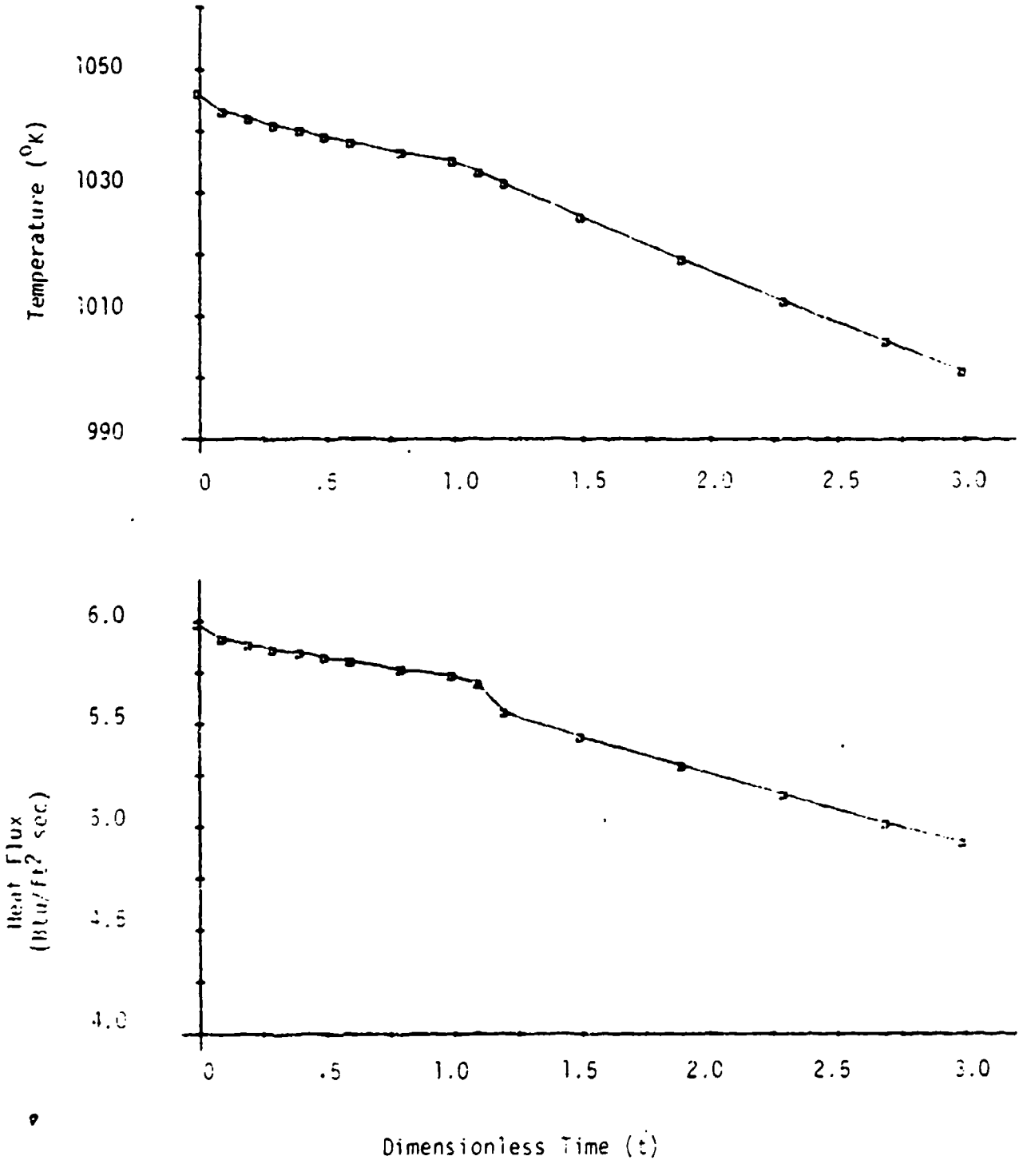
O/F = 1.02

The temperature and heat flux from a fireball that results from 1.34×10^5 pound mixture of A-50 and N_2O_4 containing a 4X excess of A-50 are shown in Figures 6 and 7, respectively. The intitial temperature was 1046^oK and decreased to 1035^oK at lift-off, $t' = 1$, which, for this case, occurs 4.3 seconds after ignition. The temperature continues to decrease after lift-off and is 1000^oK at $t' = 3$ or 12.9 seconds after ignition. The initial heat flux for this case is 6 Btu/sec ft^2 and decreases to 5.7 Btu/sec ft^2 at $t' = 1$. At $t' = 3$, the heat flux has decreased to 4.9 Btu/sec ft^2. The increased energy needed to evaporate and heat the excess A-50 reduces the energy available to raise the temperature of the fireball and radiate to the environment.

Figures 8 and 9 show the relationships of the temperature and radiant heat flux vs. time for a 2.3×10^5 pound mixture of A-50 and N_2O_4 containing a 4X excess of N_2O_4. The initial temperature of this system is 810^oK and decreases to 804^oK at lift-off, $t' = 1$ or $t = 4.7$ seconds after ignition. The temperature decreases to 786^oK at $t' = 3$ or 14.1 seconds after ignition. Again, the temperature and heat flux are decreased because of the energy needed to raise the temperature and vaporize the excess N_2O_4.

3. Conclusion

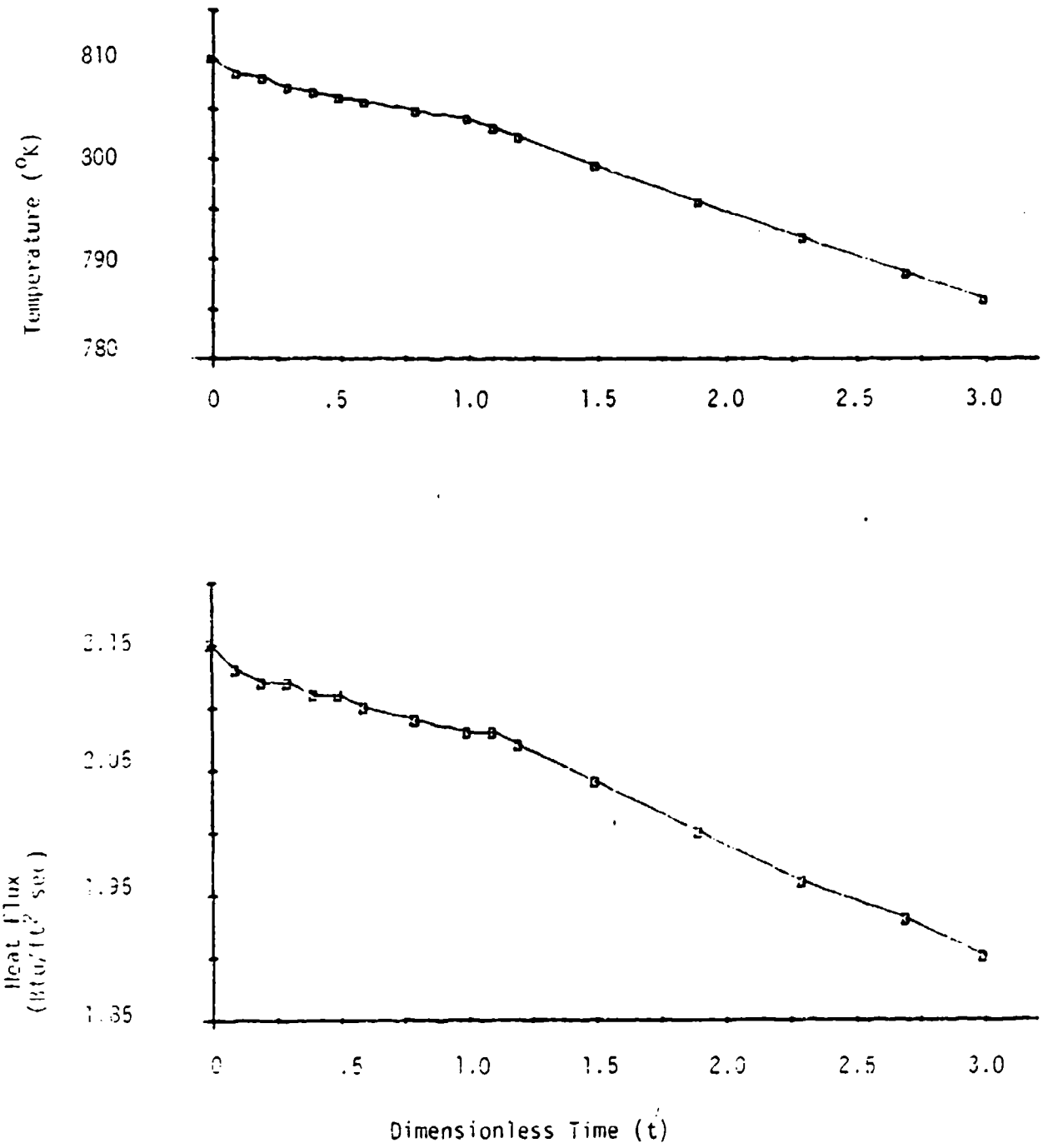
The equations developed and evaluated in this section of the report are general and can be used to determine the temperature and heat flux from a homogeneous fireball when the thermodynamic properties of the reactants and products are known. The maximum temperature and heat flux result from a stoichiometric mixing of the propellants. Excess N_2O_4 reduce both of these properties of the fireball more than excess fuel because of its greater heat of vaporization and specific heat. This causes more energy to be consumed by the components of the reaction mixture; therefore, less energy is released to the environment.



Figures 6 and 7. Radiative Fireball Temperature and Heat Loss

$W_b = 1.34 \times 10^5$ Pounds

O/F = 0.204



Figures 8 and 9. Radiative Fireball Temperature and Heat Loss

$W_b = 2.26 \times 10^5$ Pounds

O/F = 5.1

SECTION V

REACTIONS OF HYPERGOLIC PROPELLANTS WITH OTHER CHEMICALS

To characterize the explosive hazards of reacting a hypergolic fuel (A-50 or NTO) with other chemicals that may be encountered in a highway or railway accident, the NASA SP-273 computer program was used to predict the theoretical flame temperatures and combustion products resulting from such an accident. Calculations were performed, assuming an equal weight of hypergolic fuel and nonpropellant chemical (O/F weight ratio of 1.0), and were performed at 1.0 atmosphere total pressure which would be indicative of an open-field accident. Because these calculations only consider ideal chemical thermodynamic conditions (and not kinetic parameters as discussed in Section A), the computer output for these reactions contains only the combustion products which would be present at chemical equilibrium.

The chemical reactants used as computer input for these calculations are included in Table V. Computer output for the reactions of hypergolic rocket propellants with these other chemicals are included in Appendix C.

TABLE V. COMPUTER INPUT FOR REACTIONS OF HYPERGOLIC ROCKET PROPELLANTS WITH OTHER CHEMICALS

Case No.	Fuel*	Oxidant*
34	Methylene Chloride	NTO
35	Ethylene Gylcol	NTO
36	Dichlorcethane	NTO
37	Liquid Propane	NTO
38	n-Octane	NTO
39	Acetone	NTO
40	Acetylene	NTO
41	Ammonia	NTO
42	A-50	Liquid Oxygen (LOX)
43	A-50	Air (g)
44	A-50	Chlorine
45	A-50	Nitric Acid
46	A-50	Hydrogen Peroxide

* All reactants are in the liquid state unless otherwise noted.

SECTION VI
CONCLUSIONS

The purpose of this document is to provide engineering data which will be used to predict the aerial dispersion patterns of chemical reaction products resulting from catastrophic accidents involving the mixing of hypergolic liquid rocket propellants. The analysis methods described in this report have been developed for the A-50/NTO propellant combination, but the general thermodynamic methods are applicable to any other fuel/oxidizer combination which may be encountered in an accidental hypergolic vapor release. The salient features of the computational methods described in this report are:

1. Stoichiometric reactions of A-50 fuel and NTO oxidizer have been successfully characterized using the NASA SP-273 computer program for the calculation of complex chemical equilibrium and rocket performance. Reactions have been defined according to the type of propellant accident (open-field, open-silo, closed-silo, and hypergolic explosion) and according to the presence of interacting air. For a catastrophic accident involving the full inventory of liquid oxidizer (207, 560 pounds nitrogen tetroxide) and liquid fuel (104, 609 pounds Aerozine-50) which occurs in an open Titan II missile silo, the calculated adiabatic flame temperature is 2916^{o}K (5249^{o}R) which is consistent with fireball data previously reported in the literature[15]. This calculation was performed assuming thermal interaction of air present in the closed silo (125,000 ft^3 air). The major gaseous combustion products contained in the fireball were determined to be carbon monoxide, carbon dioxide, hydrogen radical, hydrogen, water vapor, nitric oxide, nitrogen, hydroxide radical, and oxygen.

2. For hypergolic combustion under nonstoichiometric conditions (O/F mole ratio $\neq$ 1.02) a calculation methodology is presented in which the heat evolved from the stoichiometric reaction was used to heat and vaporize the excess propellant. Major fireball components for the fuel-rich reaction were hydrazine vapor, UDMH vapor, nitrogen gas and

water vapor for accident scenarios which favored A-50 evaporation; and ammonia vapor, UDMH vapor, nitrogen gas, hydrogen gas, and water vapor for accidents characterized by A-50 evaporation and hydrazine monodecomposition. Fuel-lean hypergolic reactions contained both nitrogen dioxide gas and nitrogen tetroxide gas in the vapor phase of the fireball, the proportions of which depended upon the adiabatic temperature of the resultant fireball. Oxidizer to fuel mole ratios above 17.7 and below 0.06 were not characterized in this analysis, because the thermal energies derived from these hypergolic reactions were not sufficient to vaporize the excess propellant.

3. A generalized scheme for determining time-temperature and heat flux-temperature profiles for hypergolic fireballs is discussed. The development of the heat flux equations was based on the assumption that the major heat loss mechanism during fireball generation and lift-off was radiative, and conductive and convective heat losses were negligible. This is consistent with fireball heat transfer mechanisms previously reported in the literature[21]. The largest initial heat flux calculated was for the stoichiometric reaction of A-50 fuel and NTO oxidizer. This reaction gave an initial heat flux and temperature of 400 Btu/ft^2 second and 2979°K, respectively. The temperature of the fireball for this stoichiometric combustion dropped to approximately 2240°K at lift-off ($t' = 1.0$). Nonstoichiometric hypergolic combustions yielded much smaller initial heat fluxes and temperatures
($Q/A = 2.15$ Btu/ft^2 second, $T = 810$°K for $O/F = 5.1$;
$Q/A = 5.98$ Btu/ft^2 second, $T = 1046$°K for $O/F = 0.20$).
As a result, the initial adiabatic flame temperature for these nonstoichiometric hypergolic reactions did not change appreciably during fireball generation and lift-off.

4. Fireball sizes were estimated using the theoretical equations:

$$r_b = \left[\frac{3}{4\pi\rho}\right]^{1/3} W_b^{1/3}$$

Where r_b = fireball radius

W_b = total propellant weight (lbs) in reaction

ρ = density of combustion products

for an ideal gas:

$$\rho = \frac{MW_{avg}\ P}{RT_P}$$

Where MW_{avg} = average molecular weight of combustion gases

P = pressure of gases (14.7 psia under standard conditions)

R = ideal gas constant (10.731 ft^3 - psia/^oR - mole)

T_f = adiabatic flame temperature (^oR)

The calculated fireball radius for an accident involving the full inventory of A-50 fuel and NTO oxidizer (W_b = 3.12 X 10^5 pound; MW_{avg} = 21.9; T_P = 5249^oR) using this approach is approximately 235 feet which generally corresponds to the fireball radius established empirically for A-50/NTO reactions[20]:

$$r_b = 4.43\ W_b^{0.328} = 281 \text{ feet}$$

5. Computational methods using the SP-273 computer program were used to predict the thermal energies and chemical reaction products resulting from the mixing of a hypergolic liquid rocket propellant with other chemical

species that may be encountered in a highway or rail accident. Although these calculations were performed assuming ideal thermodynamic conditions for the chemical reactants and products, they are still useful for estimating fireball temperatures and hazardous vapor envelopes for these accident scenarios.

In addition to the computational methods described above for the characterization of critical fireball parameters (e.g., chemical composition, thermal energy, and geometric size), an exhaustive literature survey was completed in order to compile existing knowledge in the hydrazine (MMH, UDMH) - nitrogen tetroxide hypergolic reaction. Over 50 chemical reaction products resulting from this combination have been described in the literature, and most of these products can be accounted for by one or more simple chemical mechanisms. One of these chemical components, nitrosodimethylamine, is of particular concern in a hypergolic bipropellant accident, because it is a confirmed product in both the A-50/NTO reaction and in the A-50/air reaction, and is a known carcinogen.

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APPENDIX A

COMPUTER OUTPUT

AEROZINE-50/NITROGEN TETROXIDE REACTIONS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 1

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.95640	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.04360	-28.200	G	298.15	0.0000

D/F= 2.0760 PERCENT FUEL= 32.5098 EQUIVALENCE RATIO= 1.1157 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2916
H, CAL/G	60.7
S, CAL/(G)(K)	3.0685
M, MOL WT	21.894
(DLV/DLP)T	-1.03689
(DLV/DLT)P	1.7869
CP, CAL/(G)(K)	2.0254
GAMMA (S)	1.1188
CPF,CAL/(G)(K)	.4782
SON VEL,M/SEC	1113.2

60

MOLE FRACTIONS

AR	.00021
CO	.07225
CO2	.04519
H	.03327
HO2	.00001
H2	.07615
H2O	.34286
NO	.00977
N2	.33634
O	.01283
OH	.04666
O2	.02346

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO2	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	O	N3	O3		

NOTE WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 1

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.95640	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.04360	-28.200	G	298.15	0.0000

O/F= 2.0760 PERCENT FUEL= 32.5098 EQUIVALENCE RATIO= 1.1157 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	12.56
T, DEG K	3180
H, CAL/G	60.7
S, CAL/(G)(K)	2.8415
M, MOL WT	22.412
(DLV/DLP)T	-1.02664
(DLV/DLT)P	1.5335
CP, CAL/(G)(K)	1.4477
GAMMA (S)	1.1330
CPF,CAL/(G)(K)	.4824
SON VEL,M/SEC	1156.1

MOLE FRACTIONS

AR	.00021
CO	.06946
CO2	.05178
H	.01925
HO2	.00002
H2	.06655
H2O	.37307
N	.00001
NO	.01120
N2	.34369
O	.00726
OH	.04114
O2	.01634

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	2H	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	2H2	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
H2O(S)	H2O(L)	H2O2	NCO	NH	NH2	NH3	NO2	NO3	N2H4
N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3			

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO.

	CHEMICAL FORMULA							WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000				.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000		.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000				.95640	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C .00030	.04360	-28.200	G	298.15	0.0000

O/F= 2.0760 PERCENT FUEL= 32.5098 EQUIVALENCE RATIO= 1.1157 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	60.30
T, DEG K	3340
H, CAL/G	60.7
S, CAL/(G)(K)	2.7034
M, MOL WT	22.731
(DLV/DLP)T	-1.02075
(DLV/DLT)P	1.4026
CP, CAL/(G)(K)	1.1822
GAMMA (S)	1.1425
CPF,CAL/(G)(K)	.4848
SON VEL,M/SEC	1181.4

MOLE FRACTIONS

AR	.00022
CO	.06643
CO2	.05653
H	.01261
HNO	.00001
HO2	.00003
H2	.05947
H2O	.39304
H2O2	.00001
N	.00001
NO	.01131
NO2	.00001
N2	.34860
O	.00450
OH	.03534
O2	.01187

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	[illegible]	C5	HCN	HCO	HNCO	HNO2	HNO3	H2O(S)
H2O(L)	NCO	NH	NH2	NH3	NO3	N2H4	N2H4(L)	N2O	N2O4
N2O4(L)	N2O5	N3	O3						

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 1

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.95640	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.04360	-28.200	G	298.15	0.0000

O/F= 2.0760 PERCENT FUEL= 32.5098 EQUIVALENCE RATIO= 1.1157 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	71.90
T, DEG K	3357
H, CAL/G	60.7
S, CAL/(G)(K)	2.6880
M, MOL WT	22.766
(DLV/DLP)T	-1.02012
(DLV/DLT)P	1.3892
CP, CAL/(G)(K)	1.1562
GAMMA (S)	1.1436
CPF,CAL/(G)(K)	.4850
SON VEL,M/SEC	1184.2

MOLE FRACTIONS

AR	.00022
CO	.06603
CO2	.05712
H	.01197
HNO	.00001
HO2	.00003
H2	.05865
H2O	.12528
H2O2	.00001
N	.00001
NH2	.00001
NO	.01127
NO2	.00001
N2	.34916
O	.00424
OH	.03459
O2	.01138

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO2	HNO3	H2O(S)
H2O(L)	NCO	NH	NH3	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)
N2O5	N3	O3							

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 2

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.68660	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.31340	-28.200	G	298.15	0.0000

O/F= 2.8900 PERCENT FUEL= 25.7069 EQUIVALENCE RATIO= .9839 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2833
H, CAL/G	47.8
S, CAL/(G)(K)	2.8588
M, MOL WT	23.624
(DLV/DLP)T	-1.02779
(DLV/DLT)P	1.6163
CP, CAL/(G)(K)	1.6140
GAMMA (S)	1.1215
CPF,CAL/(G)(K)	.4414
SON VEL,M/SEC	1057.5

MOLE FRACTIONS

AR	.00177
CO	.04883
CO2	.05228
H	.01901
HO2	.00001
H2	.04329
H2O	.31854
NO	.01177
N2	.41865
O	.01133
OH	.04054
O2	.03399

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO2	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3		

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 2

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	3.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.68660	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.31340	-28.200	G	298.15	0.0000

O/F= 2.8900 PERCENT FUEL= 25.7069 EQUIVALENCE RATIO= .9839 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	12.56
T, DEG K	3062
H, CAL/G	47.8
S, CAL/(G)(K)	2.6481
M, MOL WT	24.103
(DLV/DLP)T	-1.01983
(DLV/DLT)P	1.4166
CP, CAL/(G)(K)	1.1851
GAMMA (S)	1.1361
CPF,CAL/(G)(K)	.4450
SON VEL,M/SEC	1095.5

MOLE FRACTIONS

AR	.00181
CO	.04283
CO2	.06033
H	.00976
HO2	.00002
H2	.03334
H2O	.34371
NO	.01395
NO2	.00001
N2	.42616
O	.00637
OH	.03521
O2	.02650

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO3	N2H4
N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3			

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 3

	CHEMICAL FORMULA										WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000							.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000					.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000							.18000	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030			.82000	-28.200	G	298.15	0.0000

O/F= 11.0400 PERCENT FUEL= 8.3056 EQUIVALENCE RATIO= .4503 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1801
H, CAL/G	14.8
S, CAL/(G)(K)	2.2574
M, MOL WT	27.767
(DLV/DLP)T	-1.00007
(DLV/DLT)P	1.0028
CP, CAL/(G)(K)	.3504
GAMMA (S)	1.2584
CPF,CAL/(G)(K)	.3336
SON VEL,M/SEC	823.7

MOLE FRACTIONS

AR	.00672
CO	.00002
CO2	.03857
H2	.00002
H2O	.14832
NO	.00329
NO2	.00001
N2	.66620
O	.00004
OH	.00074
O2	.13606

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	H	HCN	HCO	HNCO	HNO	HNO2
HNO3	HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3
NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3	

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 3

	CHEMICAL FORMULA										WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000							.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000					.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000							.18000	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030			.82000	-28.200	G	298.15	0.0000

O/F= 11.0400 PERCENT FUEL= 8.3056 EQUIVALENCE RATIO= .4503 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	12.56
T, DEG K	1803
H, CAL/G	14.8
S, CAL/(G)(K)	2.0763
M, MOL WT	27.771
(DLV/DLP)T	-1.00004
(DLV/DLT)P	1.0013
CP, CAL/(G)(K)	.3461
GAMMA (S)	1.2614
CPF,CAL/(G)(K)	.3336
SON VEL,M/SEC	825.0

MOLE FRACTIONS

AR	.00672
CO	.00001
CO2	.03859
H2	.00001
H2O	.14853
NO	.00331
NO2	.00002
N2	.66627
O	.00001
OH	.00040
O2	.13613

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	H	HCN	HCO	HNCO	HNO	HNO2
HNO3	HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3
NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3	

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 4

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N 2.00000	H 4.00000							.50000	12100.000	L	298.15	0.0000
FUEL	C 2.00000	H 8.00000	N 2.00000						.50000	11900.000	L	298.15	0.0000
OXIDANT	N 2.00000	O 4.00000							.02140	-4676.000	L	298.15	0.0000
OXIDANT	N 1.56176	O .41959	AR .00932	C .00030					.97860	-28.200	G	298.15	0.0000

O/F= 92.5700 PERCENT FUEL= 1.0687 EQUIVALENCE RATIO= .0713 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	536
H, CAL/G	1.1
S, CAL/(G)(K)	1.7998
M, MOL WT	28.805
(DLV/DLP)T	-1.00000
(DLV/DLT)P	1.0000
CP, CAL/(G)(K)	.2507
GAMMA (S)	1.3796
CPF,CAL/(G)(K)	.2507
SON VEL,M/SEC	462.1

MOLE FRACTIONS

AR	.00698
CO2	.00541
H2O	.01985
N2	.76584
O2	.19992

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HNCO	HNO
HNO2	HNO3	HO2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
NH2	NH3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)
N2O5	N3	O	OH	O3					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 4

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.02140	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.97860	-28.200	G	298.15	0.0000

O/F= 92.5700 PERCENT FUEL= 1.0687 EQUIVALENCE RATIO= .0713 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	12.56
T, DEG K	536
H, CAL/G	1.1
S, CAL/(G)(K)	1.6253
M, MOL WT	28.805
(DLV/DLP)T	-1.00000
(DLV/DLT)P	1.0000
CP, CAL/(G)(K)	.2507
GAMMA (S)	1.3796
CPF,CAL/(G)(K)	.2507
SON VEL,M/SEC	462.1

MOLE FRACTIONS

AR	.00898
CO2	.00541
H2O	.01985
N2	.76584
O2	.19992

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HNCO	HNO
HNO2	HNO3	HO2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
NH2	NH3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)
N2O5	N3	O	OH	O3					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 5

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.00220	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.99780	-28.200	G	298.15	0.0000

O/F=907.8000 PERCENT FUEL= .1100 EQUIVALENCE RATIO= .0088 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	323
H, CAL/G	-.8
S, CAL/(G)(K)	1.6612
M, MOL WT	28.948
(DLV/DLP)T	-1.00000
(DLV/DLT)P	1.0000
CP, CAL/(G)(K)	.2407
GAMMA (S)	1.3991
CPF,CAL/(G)(K)	.2407
SON VEL,M/SEC	360.4

MOLE FRACTIONS

AR	.00929
CO2	.00083
H2O	.00205
N2	.77932
O2	.20851

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HNCO	HNO
HNO2	HNO3	HO2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
NH2	NH3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)
N2O5	N3	O	OH	O3					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 5

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.00220	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.99780	-28.200	G	298.15	0.0000

O/F=907.8000 PERCENT FUEL= .1100 EQUIVALENCE RATIO= .0088 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	12.56
T, DEG K	323
H, CAL/G	-.8
S, CAL/(G)(K)	1.4874
M, MOL WT	28.948
(DLV/DLP)T	-1.00000
(DLV/DLT)P	1.0000
CP, CAL/(G)(K)	.2407
GAMMA (S)	1.3991
CPF,CAL/(G)(K)	.2407
SON VEL,M/SEC	360.4

MOLE FRACTIONS

AR	.00929
CO2	.00083
H2O	.00205
N2	.77932
O2	.20851

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HNCO	HNO
HNO2	HNO3	HO2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
NH2	NH3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)
N2O5	N3	O	OH	O3					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 6

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.95640	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.04360	-28.200	G	298.15	0.0000

O/F= 2.3480 PERCENT FUEL= 29.8686 EQUIVALENCE RATIO= .9864 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2907
H, CAL/G	51.8
S, CAL/(G)(K)	2.9872
M, MOL WT	22.682
(DLV/DLP)T	-1.03672
(DLV/DLT)P	1.7883
CP, CAL/(G)(K)	1.9736
GAMMA (S)	1.1176
CPF,CAL/(G)(K)	.4638
SON VEL,M/SEC	1091.3

MOLE FRACTIONS

AR	.00022
CO	.05996
CO2	.05277
H	.02746
HO2	.00001
H2	.05527
H2O	.34162
NO	.01286
N2	.33967
O	.01643
OH	.05245
O2	.04126

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO2	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3		

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 6

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.95640	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.04360	-28.200	G	298.15	0.0000

O/F= 2.3480 PERCENT FUEL= 29.8686 EQUIVALENCE RATIO= .9864 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	12.56
T, DEG K	3168
H, CAL/G	51.8
S, CAL/(G)(K)	2.7681
M, MOL WT	23.220
(DLV/DLP)T	-1.02715
(DLV/DLT)P	1.5466
CP, CAL/(G)(K)	1.4317
GAMMA (S)	1.1310
CPF,CAL/(G)(K)	.4679
SON VEL,M/SEC	1132.7

MOLE FRACTIONS

AR	.00023
CO	.05480
CO2	.06060
H	.01527
HNO	.00001
HO2	.00003
H2	.04472
H2O	.37090
H2O2	.00001
N	.00001
NO	.01585
NO2	.00001
N2	.34638
O	.01000
OH	.04790
O2	.03330

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO2	HNO3	H2O(S)
H2O(L)	NCO	NH	NH2	NH3	NO3	N2H4	N2H4(L)	N2O	N2O4
N2O4(L)	N2O5	N3	O3						

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 6

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.95640	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.04360	-28.200	G	298.15	0.0000

O/F= 2.3480 PERCENT FUEL= 29.8686 EQUIVALENCE RATIO= .9864 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	59.00
T, DEG K	3326
H, CAL/G	51.8
S, CAL/(G)(K)	2.6366
M, MOL WT	23.552
(DLV/DLP)T	-1.02189
(DLV/DLT)P	1.4260
CP, CAL/(G)(K)	1.1890
GAMMA (S)	1.1395
CPF,CAL/(G)(K)	.4703
SON VEL,M/SEC	1156.7

MOLE FRACTIONS

AR	.00023
CO	.04988
CO2	.06718
H	.00976
HNO	.00001
HO2	.00005
H2	.03737
H2O	.38989
H2O2	.00001
N	.00001
NO	.01721
NO2	.00002
N2	.35075
O	.00673
OH	.04283
O2	.02804

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO2	HNO3	H2O(S)
H2O(L)	NCO	NH	NH2	NH3	NO3	N2H4	N2H4(L)	N2O	N2O4
N2O4(L)	N2O5	N3	O3						

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 6

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000					.95640	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	.04360	-28.200	G	298.15	0.0000

O/F= 2.3480 PERCENT FUEL= 29.8686 EQUIVALENCE RATIO= .9864 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	70.60
T, DEG K	3344
H, CAL/G	51.8
S, CAL/(G)(K)	2.6215
M, MOL WT	23.590
(DLV/DLP)T	-1.02131
(DLV/DLT)P	1.4133
CP, CAL/(G)(K)	1.16e7
GAMMA (S)	1.1405
CPF,CAL/(G)(K)	.4706
SON VEL,M/SEC	1159.4

MOLE FRACTIONS

AR	.00023
CO	.04922
CO2	.06802
H	.00923
HNO	.00001
HO2	.00006
H2	.03650
H2O	.39210
H2O2	.00002
N	.00001
NO	.01733
NO2	.00002
N2	.35127
N2O	.00001
O	.00640
OH	.04215
O2	.02742

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO2	HNO3	H2O(S)
H2O(L)	NCO	NH	NH2	NH3	NO3	N2H4	N2H4(L)	N2O4	N2O4(L)
N2O5	N3	O3							

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 19

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000			1.00000	-4675.000	L	298.15	0.0000

O/F= 2.2450 PERCENT FUEL= 30.8166 EQUIVALENCE RATIO= 1.0017 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2918
H, CAL/G	53.5
S, CAL/(G)(K)	3.0162
M, MOL WT	23.448
(DLV/DLP)T	-1.03828
(DLV/DLT)P	1.8176
CP, CAL/(G)(K)	2.0417
GAMMA (S)	1.4173
CPF,CAL/(G)(K)	.4689
SON VEL,M/SEC	1098.9

MOLE FRACTIONS

CO	.06301
CO2	.05210
H	.02952
HO2	.00001
H2	.05926
H2O	.34523
NO	.01260
N2	.32797
O	.01182
OH	.05366
O2	.03980

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO2	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3		

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 19

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000

O/F= 2.2450 PERCENT FUEL= 30.8166 EQUIVALENCE RATIO= 1.0017 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	12.56
T, DEG K	3185
H, CAL/G	53.5
S, CAL/(G)(K)	2.7949
M, MOL WT	22.993
(DLV/DLP)T	-1.02844
(DLV/DLT)P	1.5687
CP, CAL/(G)(K)	1.4782
GAMMA (S)	1.1305
CPF,CAL/(G)(K)	.4731
SON VEL,M/SEC	1141.0

MOLE FRACTIONS

CO	.05825
CO2	.05965
H	.01668
HNO	.00001
HO2	.00003
H2	.04868
H2O	.37526
H2O2	.00001
N	.00001
NO	.01551
NO2	.00001
N2	.33462
O	.01028
OH	.04320
O2	.03182

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO2	HNO3	H2O(S)
H2O(L)	NCO	NH	NH2	NH3	NO3	N2H4	N2H4(L)	N2O	N2O4
N2O4(L)	N2O5	N3	O3						

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 32

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000

O/F= 1.1220 PERCENT FUEL= 47.1254 EQUIVALENCE RATIO= 2.0043 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2603
H, CAL/G	108.8
S, CAL/(G)(K)	3.4772
M, MOL WT	17.868
(DLV/DLP)T	-1.00650
(DLV/DLT)P	1.1448
CP, CAL/(G)(K)	.9134
GAMMA (S)	1.1807
CP*,CAL/(G)(K)	.5492
SON VEL,M/SEC	1195.9

MOLE FRACTIONS

CO	.12301
CO2	.01710
H	.02051
H2	.28198
H2O	.24865
NO	.00033
N2	.30395
O	.00020
OH	.00418
O2	.00007

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO2
NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3	

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 20

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	H	2.00000	I	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	3.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000

O/F= .4490 PERCENT FUEL= 69.0131 EQUIVALENCE RATIO= 5.0085 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1372
H, CAL/G	182.9
S, CAL/(G)(K)	3.8696
M, MOL WT	13.183
(DLV/DLP)T	-1.00013
(DLV/DLT)P	1.0012
CP, CAL/(G)(K)	.6087
GAMMA (S)	1.3300
CPF,CAL/(G)(K)	.6038
SON VEL,M/SEC	1072.8

MOLE FRACTIONS

CH4	.00003
CO	.14835
CO2	.00300
H2	.56334
H2O	.02323
NH3	.00002
N2	.26203

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2
C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3
C3O2	C4	C5	H	HCN	HCO	HNCO	HNO	HNO2	HNO3
HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO2
NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH
O2	O3								

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 21

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000

O/F= .2245 PERCENT FUEL= 81.6660 EQUIVALENCE RATIO= 10.0169 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1086
H, CAL/G	225.7
S, CAL/(G)(K)	3.8981
M, MOL WT	12.452
(DLV/DLP)T	-1.02078
(DLV/DLT)P	1.2432
C_P, CAL/(G)(K)	1.1252
GAMMA (S)	1.2475
CPF,CAL/(G)(K)	.6466
SON VEL,M/SEC	950.9

MOLE FRACTIONS

C(S)	.05777
CH4	.01488
CO	.08586
CO2	.00090
HCN	.00001
H2	.58210
H2O	.00585
NH3	.00008
N2	.25254

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3	C3O2
C4	C5	H	HCO	HNCO	HNO	HNO2	HNO3	HO2	H2O(S)
H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO2	NO3	N2H4
N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH	O2	O3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 23

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000

O/F= .0225 PERCENT FUEL= 97.8043 EQUIVALENCE RATIO= ******* DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	946
H, CAL/G	280.4
S, CAL/(G)(K)	3.8767
M, MOL WT	12.275
(DLV/DLP)T	-1.05380
(DLV/DLT)P	1.6248
CP, CAL/(G)(K)	1.8952
GAMMA (S)	1.2073
CPF,CAL/(G)(K)	.7043
SON VEL,M/SEC	879.3

MOLE FRACTIONS

C(S)	.10830
CH4	.06349
CO	00626
CO2	.00008
H2	.55903
H2O	.00402
NH3	.00020
N2	.25861

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3	C3O2
C4	C5	H	HCN	HCO	HNCO	HNO	HNO2	HNO3	HO2
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO2	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH	O2
O3									

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 33

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000

O/F= 4.4900 PERCENT FUEL= 18.2149 EQUIVALENCE RATIO= .5008 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2636
H, CAL/G	10.9
S, CAL/(G)(K)	2.6006
M, MOL WT	26.375
(DLV/DLP)T	-1.01134
(DLV/DLT)P	1.2783
CP, CAL/(G)(K)	.9427
GAMMA (S)	1.1354
CPF,CAL/(G)(K)	.3967
SON VEL,M/SEC	971.3

MOLE FRACTIONS

CO	.01068
CO2	.06925
H	.00364
HO2	.00002
H2	.00680
H2O	.28304
NO	.02016
NO2	.00001
N2	.33927
O	.01270
OH	.03626
O2	.21816

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO3	N2H4
N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3			

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 26

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000

O/F= 11.2300 PERCENT FUEL= 8.1766 EQUIVALENCE RATIO= .2002 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1693
H, CAL/G	-23.1
S, CAL/(G)(K)	2.2030
M, MOL WT	28.955
(DLV/DLP)T	-1.00004
(DLV/DLT)P	1.0018
CP, CAL/(G)(K)	.3368
GAMMA (S)	1.2570
CPF,CAL/(G)(K)	.3229
SON VEL,M/SEC	781.6

MOLE FRACTIONS

CO2	.03939
H2O	.15241
NO	.00296
NO2	.00001
N2	.34411
O	.00003
OH	.00051
O2	.46057

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HNCO	HNO
HNO2	HNO3	HO2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
NH2	NH3	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3
O3									

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 28

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000

O/F=112.3000 PERCENT FUEL= .8826 EQUIVALENCE RATIO= .0200 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	293
H, CAL/G	-47.8
S, CAL/(G)(K)	1.6153
M, MOL WT	30.476
(DLV/DLP)T	-1.00000
(DLV/DLT)P	1.0000
CP, CAL/(G)(K)	.2303
GAMMA (S)	1.3950
CPF,CAL/(G)(K)	.2303
SON VEL,M/SEC	334.1

MOLE FRACTIONS

CO2	.00448
H2O	.01735
N2	.33473
O2	.64345

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HNCO	HNO
HNO2	HNO3	HO2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
NH2	NH3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)
N2O5	N3	O	OH	O3					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 30

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000

O/F=******** PERCENT FUEL= .0890 EQUIVALENCE RATIO= .0020 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	97
H, CAL/G	-50.5
S, CAL/(G)(K)	1.3495
M, MOL WT	30.651
(DLV/DLP)T	-1.00001
(DLV/DLT)P	1.0001
CP, CAL/(G)(K)	.2289
GAMMA (S)	1.3952
CPF,CAL/(G)(K)	.2288
SON VEL,M/SEC	191.2

MOLE FRACTIONS

CO2	.00045
HNO3	.00001
H2O	.00176
N2	.33347
O2	.66431

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HNCO	HNO
HNO2	HO2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2
NH3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5
N3	O	OH	O3						

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

APPENDIX B

THERMOCHEMICAL CALCULATIONS FOR NONSTOICHIOMETRIC COMBUSTION OF AEROZINE-50 AND NITROGEN TETROXIDE

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 1

OXIDIZER/FUEL MOLE RATIO 1.02

PERCENT MIXING 100

VAPORIZATION CONDITIONS No Excess Propellant

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 0

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 2979 °K (5363 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.061
carbon dioxide	CO_2	.050
hydrogen radical	H	.028
hydrogen	H_2	.057
water vapor	H_2O	.332
nitric oxide	NO	.012
nitrogen	N_2	.316
hydroxide	OH	.052
oxygen	O_2	.094
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 23.13 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 2

OXIDIZER/FUEL MOLE RATIO 0.51

PERCENT MIXING 100

VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = .6545 a_{14} = .3489 a_{15} = 0

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 1975 °K (3556 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.052
carbon dioxide	CO_2	.043
hydrogen radical	H	.024
hydrogen	H_2	.049
water vapor	H_2O	.286
nitric oxide	NO	.010
nitrogen	N_2	.272
hydroxide	OH	.045
oxygen	O_2	.081
hydrazine vapor	$N_2H_4(g)$	.090
UDMH vapor	$C_2H_8N_2(g)$	.048
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 25.66 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 3

OXIDIZER/FUEL MOLE RATIO .51

PERCENT MIXING 100

VAPORIZATION CONDITIONS UDMH Selective Evaporation

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = .3489 a_{15} = 0

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 2402 °K (4324 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.057
carbon dioxide	CO_2	.047
hydrogen radical	H	.026
hydrogen	H_2	.054
water vapor	H_2O	.314
nitric oxide	NO	.011
nitrogen	N_2	.299
hydroxide	OH	.049
oxygen	O_2	.089
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.053
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 25.02 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 4

OXIDIZER/FUEL MOLE RATIO .51

PERCENT MIXING 100

VAPORIZATION CONDITIONS UDMH Evaporation & Hydrazine Decomposition

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = .3489 a_{15} = 0

a_{16} = .6545 a_{17} = .3272 a_{18} = .3272

a_{19} = 0

RESULTS:

Flame Temperature 2239 °K (4031 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.048
carbon dioxide	CO_2	.040
hydrogen radical	H	.022
hydrogen	H_2	.086
water vapor	H_2O	.263
nitric oxide	NO	.009
nitrogen	N_2	.291
hydroxide	OH	.041
oxygen	O_2	.074
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.044
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.082
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 23.55 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 5

OXIDIZER/FUEL MOLE RATIO .204

PERCENT MIXING 100

VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 2.614 a_{14} = 1.394 a_{15} = 0

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 1046 °K (1882 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.037
carbon dioxide	CO_2	.031
hydrogen radical	H	.017
hydrogen	H_2	.035
water vapor	H_2O	.203
nitric oxide	NO	.007
nitrogen	N_2	.193
hydroxide	OH	.032
oxygen	O_2	.057
hydrazine vapor	$N_2H_4(g)$	.254
UDMH vapor	$C_2H_8N_2(g)$	.135
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 30.38 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 6

OXIDIZER/FUEL MOLE RATIO .204

PERCENT MIXING 100

VAPORIZATION CONDITIONS UDMH Evaporation & Hydrazine Decomposition

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 1.394 a_{15} = 0

a_{16} = 2.614 a_{17} = 1.307 a_{18} = 1.307

a_{19} = 0

RESULTS:

Flame Temperature 1523 °K (2742 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.029
carbon dioxide	CO_2	.024
hydrogen radical	H	.014
hydrogen	H_2	.129
water vapor	H_2O	.162
nitric oxide	NO	.006
nitrogen	N_2	.255
hydroxide	OH	.025
oxygen	O_2	.046
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.108
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.202
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 24.20 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 7

OXIDIZER/FUEL MOLE RATIO .102

PERCENT MIXING 100

VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 5.881 a_{14} = 3.136 a_{15} = 0

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 580 °K (1045 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.025
carbon dioxide	CO_2	.021
hydrogen radical	H	.011
hydrogen	H_2	.023
water vapor	H_2O	.136
nitric oxide	NO	.005
nitrogen	N_2	.130
hydroxide	OH	.021
oxygen	O_2	.039
hydrazine vapor	$N_2H_4(g)$	.384
UDMH vapor	$C_2H_8N_2(g)$	.205
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 34.06 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 8

OXIDIZER/FUEL MOLE RATIO .102

PERCENT MIXING 100

VAPORIZATION CONDITIONS UDMH Evaporation & Hydrazine Decomposition

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 3.136 a_{15} = 0

a_{16} = 5.881 a_{17} = 2.941 a_{18} = 2.941

a_{19} = 0

RESULTS:

Flame Temperature 1206 °K (2171 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.018
carbon dioxide	CO_2	.015
hydrogen radical	H	.008
hydrogen	H_2	.156
water vapor	H_2O	.098
nitric oxide	NO	.003
nitrogen	N_2	.232
hydroxide	OH	.015
oxygen	O_2	.028
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.148
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.278
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 24.61 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 9

OXIDIZER/FUEL MOLE RATIO .060

PERCENT MIXING 100

VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 10.39 a_{14} = 5.54 a_{15} = 0

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 298 °K (537 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.017
carbon dioxide	CO_2	.014
hydrogen radical	H	.008
hydrogen	H_2	.016
water vapor	H_2O	.094
nitric oxide	NO	.003
nitrogen	N_2	.089
hydroxide	OH	.015
oxygen	O_2	.027
hydrazine vapor	$N_2H_4(g)$	.468
UDMH vapor	$C_2H_8N_2(g)$	.249
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 36.49 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 10

OXIDIZER/FUEL MOLE RATIO .060

PERCENT MIXING 80

VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 8.31 a_{14} = 4.43 a_{15} = 0

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 406 °K (731 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.020
carbon dioxide	CO_2	.017
hydrogen radical	H	.009
hydrogen	H_2	.019
water vapor	H_2O	.110
nitric oxide	NO	.004
nitrogen	N_2	.104
hydroxide	OH	.017
oxygen	O_2	.031
hydrazine vapor	$N_2H_4(g)$	.437
UDMH vapor	$C_2H_8N_2(g)$	.233
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 35.86 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 11

OXIDIZER/FUEL MOLE RATIO .060

PERCENT MIXING 60

VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 6.23 a_{14} = 3.32 a_{15} = 0

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 550 °K (991 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.024
carbon dioxide	CO_2	.020
hydrogen radical	H	.011
hydrogen	H_2	.023
water vapor	H_2O	.132
nitric oxide	NO	.005
nitrogen	N_2	.125
hydroxide	OH	.021
oxygen	O_2	.037
hydrazine vapor	$N_2H_4(g)$	.393
UDMH vapor	$C_2H_8N_2(g)$	.210
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 34.39 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 12

OXIDIZER/FUEL MOLE RATIO .060

PERCENT MIXING 40

VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 4.16 a_{14} = 2.22 a_{15} = 0

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 769 °K (1385 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.030
carbon dioxide	CO_2	.025
hydrogen radical	H	.014
hydrogen	H_2	.028
water vapor	H_2O	.166
nitric oxide	NO	.006
nitrogen	N_2	.157
hydroxide	OH	.026
oxygen	O_2	.047
hydrazine vapor	$N_2H_4(g)$	.328
UDMH vapor	$C_2H_8N_2(g)$	.176
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 32.62 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 13

OXIDIZER/FUEL MOLE RATIO .060

PERCENT MIXING 20

VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 2.08 a_{14} = 1.11 a_{15} = 0

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 1202 °K (2164 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.040
carbon dioxide	CO_2	.033
hydrogen radical	H	.019
hydrogen	H_2	.038
water vapor	H_2O	.220
nitric oxide	NO	.008
nitrogen	N_2	.209
hydroxide	OH	.034
oxygen	O_2	.062
hydrazine vapor	$N_2H_4(g)$	.219
UDMH vapor	$C_2H_8N_2(g)$	.117
nitrogen dioxide	NO_2	.000
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 29.33 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 14

OXIDIZER/FUEL MOLE RATIO 2.04

PERCENT MIXING 100

VAPORIZATION CONDITIONS Excess N_2O_4 (1) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 1.02

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 1958 °K (3525 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.046
carbon dioxide	CO_2	.038
hydrogen radical	H	.021
hydrogen	H_2	.043
water vapor	H_2O	.251
nitric oxide	NO	.009
nitrogen	N_2	.238
hydroxide	OH	.039
oxygen	O_2	.071
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.245
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 28.72 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 15

OXIDIZER/FUEL MOLE RATIO 5.1

PERCENT MIXING 100

VAPORIZATION CONDITIONS Excess N_2O_4 (1)100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 4.0783

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 810 °K (1459 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.026
carbon dioxide	CO_2	.022
hydrogen radical	H	.012
hydrogen	H_2	.025
water vapor	H_2O	.144
nitric oxide	NO	.005
nitrogen	N_2	.137
hydroxide	OH	.022
oxygen	O_2	.041
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.565
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 36.01 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 16

OXIDIZER/FUEL MOLE RATIO 7.00

PERCENT MIXING 100

VAPORIZATION CONDITIONS Excess N_2O_4 (l) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 5.98

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 486 °K (875 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.021
carbon dioxide	CO_2	.017
hydrogen radical	H	.010
hydrogen	H_2	.020
water vapor	H_2O	.114
nitric oxide	NO	.004
nitrogen	N_2	.109
hydroxide	OH	.018
oxygen	O_2	.032
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.656
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 38.07 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 17

OXIDIZER/FUEL MOLE RATIO 7.00

PERCENT MIXING 80

VAPORIZATION CONDITIONS Excess N_2O_4 (1) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 4.78

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 674 °K (1214 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.024
carbon dioxide	CO_2	.020
hydrogen radical	H	.011
hydrogen	H_2	.023
water vapor	H_2O	.132
nitric oxide	NO	.005
nitrogen	N_2	.125
hydroxide	OH	.021
oxygen	O_2	.037
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.603
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 36.91 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 18

OXIDIZER/FUEL MOLE RATIO 7.00

PERCENT MIXING 60

VAPORIZATION CONDITIONS Excess N_2O_4 (l) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 3.59

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 920 °K (1657 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.028
carbon dioxide	CO_2	.023
hydrogen radical	H	.013
hydrogen	H_2	.027
water vapor	H_2O	.155
nitric oxide	NO	.005
nitrogen	N_2	.147
hydroxide	OH	.024
oxygen	O_2	.044
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.533
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 35.25 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 19

OXIDIZER/FUEL MOLE RATIO 7.00

PERCENT MIXING 40

VAPORIZATION CONDITIONS Excess N_2O_4 (l) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 2.39

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 1267 °K (2281 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.034
carbon dioxide	CO_2	.028
hydrogen radical	H	.016
hydrogen	H_2	.032
water vapor	H_2O	.189
nitric oxide	NO	.007
nitrogen	N_2	.179
hydroxide	OH	.030
oxygen	O_2	.053
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.432
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 32.97 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 20

OXIDIZER/FUEL MOLE RATIO 7.00

PERCENT MIXING 20

VAPORIZATION CONDITIONS Excess N_2O_4 (1) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 1.20

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 0

RESULTS:

Flame Temperature 1840 °K (3313 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.044
carbon dioxide	CO_2	.036
hydrogen radical	H	.020
hydrogen	H_2	.041
water vapor	H_2O	.240
nitric oxide	NO	.008
nitrogen	N_2	.228
hydroxide	OH	.038
oxygen	O_2	.068
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.276
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.000

Average Molecular Weight 29.38 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 21

OXIDIZER/FUEL MOLE RATIO 8.549

PERCENT MIXING 100

VAPORIZATION CONDITIONS Excess N_2O_4 (l) 88% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 6.59

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = .93

RESULTS:

Flame Temperature 361 °K (650 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.019
carbon dioxide	CO_2	.015
hydrogen radical	H	.009
hydrogen	H_2	.017
water vapor	H_2O	.102
nitric oxide	NO	.004
nitrogen	N_2	.097
hydroxide	OH	.016
oxygen	O_2	.029
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.646
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.046

Average Molecular Weight 41.06 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 22

OXIDIZER/FUEL MOLE RATIO 13.02

PERCENT MIXING 100

VAPORIZATION CONDITIONS Excess N_2O_4 (1) 40% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 4.84

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 7.16

RESULTS:

Flame Temperature 319 °K (575 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.016
carbon dioxide	CO_2	.014
hydrogen radical	H	.008
hydrogen	H_2	.015
water vapor	H_2O	.090
nitric oxide	NO	.003
nitrogen	N_2	.086
hydroxide	OH	.014
oxygen	O_2	.026
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.418
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.310

Average Molecular Weight 54.04 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 23

OXIDIZER/FUEL MOLE RATIO 17.72

PERCENT MIXING 100

VAPORIZATION CONDITIONS Excess N_2O_4 (1) 18% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a_{13} = 0 a_{14} = 0 a_{15} = 2.97

a_{16} = 0 a_{17} = 0 a_{18} = 0

a_{19} = 13.73

RESULTS:

Flame Temperature 296 °K (533 °R)

Fireball Species	Formula	Mole Fraction
carbon monoxide	CO	.015
carbon dioxide	CO_2	.012
hydrogen radical	H	.007
hydrogen	H_2	.014
water vapor	H_2O	.080
nitric oxide	NO	.003
nitrogen	N_2	.076
hydroxide	OH	.013
oxygen	O_2	.023
hydrazine vapor	$N_2H_4(g)$	.000
UDMH vapor	$C_2H_8N_2(g)$	.000
nitrogen dioxide	NO_2	.229
ammonia	$NH_3(g)$	.000
nitrogen tetroxide	$N_2O_4(g)$	.529

Average Molecular Weight 64.80 lbs/lb-mole

APPENDIX C

COMPUTER OUTPUT, REACTIONS OF LIQUID ROCKET PROPELLANTS WITH OTHER CHEMICALS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 34

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000
FUEL	C	1.00000	H	2.00000	CL	2.00000	1.00000	-28000.000	L	298.15	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= .6393 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2325
H, CAL/G	-190.2
S, CAL/(G)(K)	1.9486
M, MOL WT	34.423
(DLV/DLP)T	-1.00839
(DLV/DLT)P	1.1775
CP, CAL/(G)(K)	.5299
GAMMA (S)	1.1664
CPF,CAL/(G)(K)	.2828
SON VEL,M/SEC	809.3

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MOLE FRACTIONS

CO	.00704
CO2	.19561
CL	.11539
CLO	.00053
CL2	.00292
H	.00021
HCL	.28355
H2	.00037
H2O	.05769
NO	.00682
NO2	.00001
N2	.18365
O	.00212
OH	.00540
O2	.13870

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CCL	CCL2	CCL3	CCL4	CH	CH2	CH2O	CH3
CH4	CN	CNN	CN2	COCL	COCL2	C2	C2CL2	C2H	C2H2
C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3	C3O2	C4
C5	CLCN	CLO2	CL2O	HCN	HCO	HNCO	HNO	HNO2	HNO3
HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NOCL
NO2CL	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 35

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000
FUEL	C	2.00000	H	6.00000	O	2.00000	1.00000	-108580.000	L	298.15	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 1.4899 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2215
H, CAL/G	-900.1
S, CAL/(G)(K)	2.9664
M, MOL WT	21.840
(DLV/DLP)T	-1.00083
(DLV/DLT)P	1.0219
CP, CAL/(G)(K)	.5497
GAMMA (S)	1.2078
CPF, CAL/(G)(K)	.4888
SON VEL, M/SEC	1009.2

MOLE FRACTIONS

CO	.24468
CO2	.10719
H	.00243
H2	.15950
H2O	.36670
NO	.00003
N2	.11867
O	.00001
OH	.00079
O2	.00001

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO2
N2?	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3	

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 36

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000
FUEL	C	2.00000	H	4.00000	CL	2.00000	1.00000	-39700.000	L	298.15	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 1.1316 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2744
H, CAL/G	-226.0
S, CAL/(G)(K)	2.2532
M, MOL WT	30.337
(DLV/DLP)T	-1.02720
(DLV/DLT)P	1.6036
CP, CAL/(G)(K)	1.2256
GAMMA (S)	1.1239
CPF,CAL/(G)(K)	.3314
SON VEL,M/SEC	919.4

MOLE FRACTIONS

CO	.15673
CO2	.14982
CL	.07058
CLO	.00008
CL2	.00014
H	.01025
HCL	.23560
H2	.02369
H2O	.15121
NO	.00397
N2	.16287
O	.00486
OH	.01745
O2	.01273

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CCL	CCL2	CCL3	CCL4	CH	CH2	CH2O	CH3
CH4	CN	CNN	CN2	COCL	COCL2	C2	C2CL2	C2H	C2H2
C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3	C3O2	C4
C5	CLCN	CLO2	CL2O	HCN	HCO	HNCO	HNO	HNO2	HNO3
HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NOCL
NO2	NO2CL	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3
O3									

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 37

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	N	2.00000	O	4.00000	1.00000	-4676.000	L	298.15	0.0000
FUEL	C	3.00000	H	8.00000	1.00000	-30372.000	L	231.00	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 5.2164 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1013
H, CAL/G	-369.8
S, CAL/(G)(K)	3.3318
M, MOL WT	15.142
(DLV/DLP)T	-1.06793
(DLV/DLT)P	2.0262
CP, CAL/(G)(K)	2.7647
GAMMA (S)	1.1454
CPF,CAL/(G)(K)	.6056
SON VEL,M/SEC	798.2

MOLE FRACTIONS

C(S)	.18445
CH4	.02359
CO	.19196
CO2	.02006
H2	.47646
H2O	.03635
NH3	.00006
N2	.06708

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3	C3O2
C4	C5	H	HCN	HCO	HNCO	HNO	HNO2	HNO3	HO2
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO2	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH	O2
O3									

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 38

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	N	2.00000	O	4.00000	1.00000	-4676.000	L	298.15	0.0000
FUEL	C	8.00000	H	18.00000	1.00000	-59740.000	L	298.15	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 5.0342 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1057
H, CAL/G	-286.9
S, CAL/(G)(K)	3.2004
M, MOL WT	15.922
(DLV/DLP)T	-1.04810
(DLV/DLT)P	1.7106
CP, CAL/(G)(K)	1.9567
GAMMA (S)	1.1608
CPF,CAL/(G)(K)	.5728
SON VEL,M/SEC	800.6

MOLE FRACTIONS

C(S)	.19137
CH4	.01398
CO	.23277
CO2	.01271
H2	.45751
H2O	.02166
NH3	.00004
N2	.06994

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3	C3O2
C4	C5	H	HCN	HCO	HNCO	HNO	HNO2	HNO3	HO2
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO2	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH	O2
O3									

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 39

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	N	2.00000	O	4.00000			1.00000	-4676.000	L	298.15	0.0000
FUEL	C	3.00000	H	6.00000	O	1.00000	1.00000	-59320.000	L	298.15	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 2.5532 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1276
H, CAL/G	-536.1
S, CAL/(G)(K)	3.0759
M, MOL WT	17.520
(DLV/DLP)T	-1.00025
(DLV/DLT)P	1.0028
CP, CAL/(G)(K)	.4899
GAMMA (S)	1.3031
CPF,CAL/(G)(K)	.4684
SON VEL,M/SEC	888.4

MOLE FRACTIONS

CH4	.00006
CO	.42175
CO2	.03066
H2	.40375
H2O	.04858
NH3	.00001
N2	.09520

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2
C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3
C3O2	C4	C5	H	HCN	HCO	HNCO	HNO	HNO2	HNO3
HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO2
NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH
O2	O3								

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 40

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	N 2.00000	O	4.00000		1.00000	-4676.000	L	298.15	0.0000
FUEL	C 2.00000	H	2.00000		1.00000	49270.000	L	192.50	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 4.4171 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2895
H, CAL/G	920.7
S, CAL/(G)(K)	3.0852
M, MOL WT	20.797
(DLV/DLP)T	-1.01737
(DLV/DLT)P	1.3508
CP, CAL/(G)(K)	1.4472
GAMMA (S)	1.1150
CPF,CAL/(G)(K)	.5115
SON VEL,M/SEC	1135.9

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MOLE FRACTIONS

C(S)	.21193
C	.00002
CH	.00001
CH2	.00001
CH3	.00003
CH4	.00001
CN	.00053
CO	.35624
C2	.00001
C2H	.00437
C2H2	.01388
C2N	.00013
C2N2	.00004
C3	.00007
H	.05092
HCN	.02359
H2	.26132
N2	.07689

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

CH2O	CNN	CN2	CO2	C2H4	C2H6	C2N2H8(L)	C2N2H8	C2O	C3O2
C4	C5	HCO	HNCO	HNO	HNO2	HNO3	HO2	H2O(S)	H2O(L)
H2O	H2O2	N	NCO	NH	NH2	NH3	NO	NO2	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH	O2
O3									

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 41

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	N	2.00000	O	4.00000	1.00000	-4676.000	L	298.15	0.0000
FUEL	N	1.00000	H	3.00000	1.00000	-17030.000	L	239.00	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 2.0260 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1674
H, CAL/G	-525.4
S, CAL/(G)(K)	3.6209
M, MOL WT	15.588
(DLV/DLP)T	-1.00002
(DLV/DLT)P	1.0006
CP, CAL/(G)(K)	.6003
GAMMA (S)	1.2700
CPF,CAL/(G)(K)	.5979
SON VEL,M/SEC	1064.8

MOLE FRACTIONS

H	.00007
H2	.34759
H2O	.33882
N2	.31352

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

HNO	HNO2	HNO3	HO2	H2O(S)	H2O(L)	H2O2	N	NH	NH2
NH3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5
N3	O	OH	O2	O3					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 42

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	O	2.00000					1.00000	-3102.000	L	90.18	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 1.5641 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2923
H, CAL/G	95.4
S, CAL/(G)(K)	3.5798
M, MOL WT	18.045
(DLV/DLP)T	-1.02928
(DLV/DLT)P	1.6086
CP CAL/(G)(K)	1.9817
GAMMA (S)	1.1293
CP,CAL/(G)(K)	.5703
SON VEL,M/SEC	1233.2

MOLE FRACTIONS

CO	.12091
CO2	.02921
H	.05493
H2	.19955
H2O	.34012
NO	.00304
N2	.21431
O	.00508
OH	.02932
O2	.00351

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO2
NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3	

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 43

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000					.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000			.50000	11900.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	AR	.00932	C	.00030	1.00000	-28.200	G	298.15	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 6.7500 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1072
H, CAL/G	143.4
S, CAL/(G)(K)	3.2190
M, MOL WT	15.653
(DLV/DLP)T	-1.01687
(DLV/DLT)P	1.2123
CP, CAL/(G)(K)	.8596
GAMMA (S)	1.2503
CPF,CAL/(G)(K)	.4997
SON VEL,M/SEC	843.9

MOLE FRACTIONS

AP	.00248
C(S)	.01420
CH4	.01048
CO	.10224
CO2	.00154
HCN	.00001
H2	.46998
H2O	.00646
NH3	.00008
N2	.39254

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3	C3O2
C4	C5	H	HCO	HNCO	HNO	HNO2	HNO3	HO2	H2O(S)
H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO2	NO3	N2H4
N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH	O2	O3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 44

	CHEMICAL FORMULA	WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N 2.00000 H 4.00000	.50000	12100.000	L	298.15	0.0000
FUEL	C 2.00000 H 8.00000 N 2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	CL 2.00000	1.00000	-5391.000	L	239.09	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 6.9319 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1318
H, CAL/G	105.9
S, CAL/(G)(K)	2.6769
M, MOL WT	19.543
(DLV/DLP)T	-1.00166
(DLV/DLT)P	1.0139
CP, CAL/(G)(K)	.4587
GAMMA (S)	1.2924
CPF,CAL/(G)(K)	.4455
SON VEL,M/SEC	851.2

MOLE FRACTIONS

C(S)	.13856
CH4	.00143
HCL	.23743
HCN	.00007
H2	.42117
NH3	.00002
N2	.20133

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .00005 FOR ALL ASSIGNED CONDITIONS

C	CCL	CCL2	CCL3	CCL4	CH	CH2	CH3	CN	CNN
CN2	C2	C2CL2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)
C2N2H8	C3	C4	C5	CL	CLCN	CL2	H	N	NH
NH2	N2H4	N2H4(L)	N3						

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 45

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	H	1.00000	N	1.00000	O	3.00000	1.00000	-41460.000	L	298.15	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 2.2201 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	2123
H, CAL/G	-185.1
S, CAL/(G)(K)	3.5836
M, MOL WT	16.521
(DLV/DLP)T	-1.00058
(DLV/DLT)P	1.0152
CP, CAL/(G)(K)	.6272
GAMMA (S)	1.2455
CPF,CAL/(G)(K)	.5755
SON VEL,M/SEC	1153.5

MOLE FRACTIONS

CO	.12108
CO2	.01637
H	.00213
H2	.35779
H2O	.23929
NO	.00001
N2	.26316
OH	.00017

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO2
NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	O2
O3									

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 46

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			.50000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	N	2.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	H	2.00000	O	2.00000			1.00000	-44860.000	L	298.15	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 2.1627 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM	1.000
T, DEG K	1939
H, CAL/G	-515.5
S, CAL/(G)(K)	3.8849
M, MOL WT	14.871
(DLV/DLP)T	-1.00015
(DLV/DLT)P	1.0051
CP, CAL/(G)(K)	.6665
GAMMA (S)	1.2537
CPF,CAL/(G)(K)	.6419
SON VEL,M/SEC	1165.9

MOLE FRACTIONS

CO	.10569
CO2	.01803
H	.00067
H2	.40230
H2O	.29539
N2	.17787
OH	.00004

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO	HNO2	HNO3
HO2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO
NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O
O2	O3								

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

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